



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:42 AM UTC

PDB ID : 4MLB / pdb\_00004mlb  
Title : Reverse polarity of binding pocket suggests different function of a MOP superfamily transporter from *Pyrococcus furiosus* Vc1 (DSM3638)  
Authors : Malviya, V.N.; Nonaka, T.; Muenke, C.; Koepke, J.; Michel, H.  
Deposited on : 2013-09-06  
Resolution : 2.35 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](mailto: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>.

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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

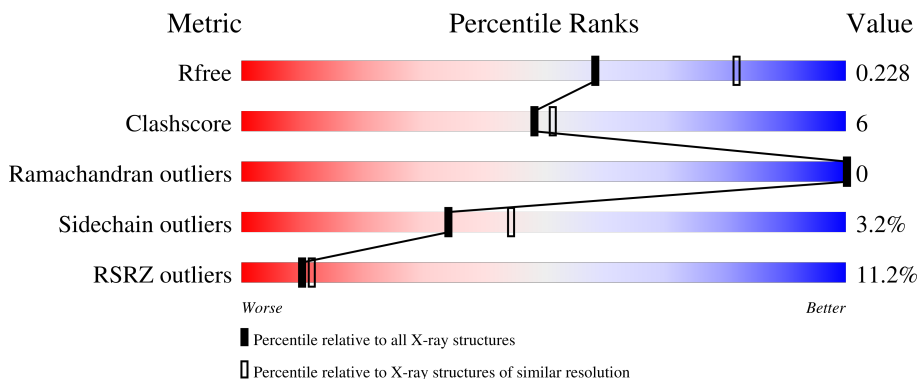
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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  $\geq 3$ , 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	492	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">8%      80%      11%      •      8%</p>
1	B	492	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7%      82%      10%      8%</p>
1	C	492	<div style="display: flex; align-items: center;"> <div style="width: 15%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">15%      80%      11%      •      8%</p>
1	D	492	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">11%      79%      12%      •      8%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CXE	B	509	-	-	-	X
2	CXE	B	511	-	-	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 14749 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 PF0708.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	453	3412	2237	557	597	21	0	1	0
1	B	454	3413	2237	555	600	21	0	0	0
1	C	452	3418	2241	559	597	21	0	2	0
1	D	452	3418	2241	559	597	21	0	2	0

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP Q8U2X0
A	-5	GLY	-	expression tag	UNP Q8U2X0
A	-4	GLY	-	expression tag	UNP Q8U2X0
A	-3	SER	-	expression tag	UNP Q8U2X0
A	-2	GLU	-	expression tag	UNP Q8U2X0
A	-1	ILE	-	expression tag	UNP Q8U2X0
A	0	PRO	-	expression tag	UNP Q8U2X0
A	298	THR	ALA	conflict	UNP Q8U2X0
A	462	ARG	-	expression tag	UNP Q8U2X0
A	463	ASN	-	expression tag	UNP Q8U2X0
A	464	SER	-	expression tag	UNP Q8U2X0
A	465	GLU	-	expression tag	UNP Q8U2X0
A	466	ASN	-	expression tag	UNP Q8U2X0
A	467	LEU	-	expression tag	UNP Q8U2X0
A	468	TYR	-	expression tag	UNP Q8U2X0
A	469	PHE	-	expression tag	UNP Q8U2X0
A	470	GLN	-	expression tag	UNP Q8U2X0
A	471	GLY	-	expression tag	UNP Q8U2X0
A	472	GLY	-	expression tag	UNP Q8U2X0
A	473	ARG	-	expression tag	UNP Q8U2X0
A	474	GLY	-	expression tag	UNP Q8U2X0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	475	SER	-	expression tag	UNP Q8U2X0
A	476	HIS	-	expression tag	UNP Q8U2X0
A	477	HIS	-	expression tag	UNP Q8U2X0
A	478	HIS	-	expression tag	UNP Q8U2X0
A	479	HIS	-	expression tag	UNP Q8U2X0
A	480	HIS	-	expression tag	UNP Q8U2X0
A	481	HIS	-	expression tag	UNP Q8U2X0
A	482	HIS	-	expression tag	UNP Q8U2X0
A	483	HIS	-	expression tag	UNP Q8U2X0
A	484	HIS	-	expression tag	UNP Q8U2X0
A	485	HIS	-	expression tag	UNP Q8U2X0
B	-6	MET	-	expression tag	UNP Q8U2X0
B	-5	GLY	-	expression tag	UNP Q8U2X0
B	-4	GLY	-	expression tag	UNP Q8U2X0
B	-3	SER	-	expression tag	UNP Q8U2X0
B	-2	GLU	-	expression tag	UNP Q8U2X0
B	-1	ILE	-	expression tag	UNP Q8U2X0
B	0	PRO	-	expression tag	UNP Q8U2X0
B	298	THR	ALA	conflict	UNP Q8U2X0
B	462	ARG	-	expression tag	UNP Q8U2X0
B	463	ASN	-	expression tag	UNP Q8U2X0
B	464	SER	-	expression tag	UNP Q8U2X0
B	465	GLU	-	expression tag	UNP Q8U2X0
B	466	ASN	-	expression tag	UNP Q8U2X0
B	467	LEU	-	expression tag	UNP Q8U2X0
B	468	TYR	-	expression tag	UNP Q8U2X0
B	469	PHE	-	expression tag	UNP Q8U2X0
B	470	GLN	-	expression tag	UNP Q8U2X0
B	471	GLY	-	expression tag	UNP Q8U2X0
B	472	GLY	-	expression tag	UNP Q8U2X0
B	473	ARG	-	expression tag	UNP Q8U2X0
B	474	GLY	-	expression tag	UNP Q8U2X0
B	475	SER	-	expression tag	UNP Q8U2X0
B	476	HIS	-	expression tag	UNP Q8U2X0
B	477	HIS	-	expression tag	UNP Q8U2X0
B	478	HIS	-	expression tag	UNP Q8U2X0
B	479	HIS	-	expression tag	UNP Q8U2X0
B	480	HIS	-	expression tag	UNP Q8U2X0
B	481	HIS	-	expression tag	UNP Q8U2X0
B	482	HIS	-	expression tag	UNP Q8U2X0
B	483	HIS	-	expression tag	UNP Q8U2X0
B	484	HIS	-	expression tag	UNP Q8U2X0

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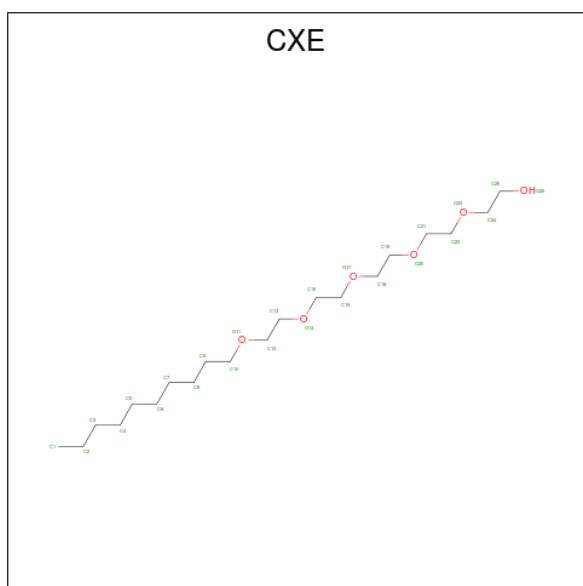
Chain	Residue	Modelled	Actual	Comment	Reference
B	485	HIS	-	expression tag	UNP Q8U2X0
C	-6	MET	-	expression tag	UNP Q8U2X0
C	-5	GLY	-	expression tag	UNP Q8U2X0
C	-4	GLY	-	expression tag	UNP Q8U2X0
C	-3	SER	-	expression tag	UNP Q8U2X0
C	-2	GLU	-	expression tag	UNP Q8U2X0
C	-1	ILE	-	expression tag	UNP Q8U2X0
C	0	PRO	-	expression tag	UNP Q8U2X0
C	298	THR	ALA	conflict	UNP Q8U2X0
C	462	ARG	-	expression tag	UNP Q8U2X0
C	463	ASN	-	expression tag	UNP Q8U2X0
C	464	SER	-	expression tag	UNP Q8U2X0
C	465	GLU	-	expression tag	UNP Q8U2X0
C	466	ASN	-	expression tag	UNP Q8U2X0
C	467	LEU	-	expression tag	UNP Q8U2X0
C	468	TYR	-	expression tag	UNP Q8U2X0
C	469	PHE	-	expression tag	UNP Q8U2X0
C	470	GLN	-	expression tag	UNP Q8U2X0
C	471	GLY	-	expression tag	UNP Q8U2X0
C	472	GLY	-	expression tag	UNP Q8U2X0
C	473	ARG	-	expression tag	UNP Q8U2X0
C	474	GLY	-	expression tag	UNP Q8U2X0
C	475	SER	-	expression tag	UNP Q8U2X0
C	476	HIS	-	expression tag	UNP Q8U2X0
C	477	HIS	-	expression tag	UNP Q8U2X0
C	478	HIS	-	expression tag	UNP Q8U2X0
C	479	HIS	-	expression tag	UNP Q8U2X0
C	480	HIS	-	expression tag	UNP Q8U2X0
C	481	HIS	-	expression tag	UNP Q8U2X0
C	482	HIS	-	expression tag	UNP Q8U2X0
C	483	HIS	-	expression tag	UNP Q8U2X0
C	484	HIS	-	expression tag	UNP Q8U2X0
C	485	HIS	-	expression tag	UNP Q8U2X0
D	-6	MET	-	expression tag	UNP Q8U2X0
D	-5	GLY	-	expression tag	UNP Q8U2X0
D	-4	GLY	-	expression tag	UNP Q8U2X0
D	-3	SER	-	expression tag	UNP Q8U2X0
D	-2	GLU	-	expression tag	UNP Q8U2X0
D	-1	ILE	-	expression tag	UNP Q8U2X0
D	0	PRO	-	expression tag	UNP Q8U2X0
D	298	THR	ALA	conflict	UNP Q8U2X0
D	462	ARG	-	expression tag	UNP Q8U2X0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	463	ASN	-	expression tag	UNP Q8U2X0
D	464	SER	-	expression tag	UNP Q8U2X0
D	465	GLU	-	expression tag	UNP Q8U2X0
D	466	ASN	-	expression tag	UNP Q8U2X0
D	467	LEU	-	expression tag	UNP Q8U2X0
D	468	TYR	-	expression tag	UNP Q8U2X0
D	469	PHE	-	expression tag	UNP Q8U2X0
D	470	GLN	-	expression tag	UNP Q8U2X0
D	471	GLY	-	expression tag	UNP Q8U2X0
D	472	GLY	-	expression tag	UNP Q8U2X0
D	473	ARG	-	expression tag	UNP Q8U2X0
D	474	GLY	-	expression tag	UNP Q8U2X0
D	475	SER	-	expression tag	UNP Q8U2X0
D	476	HIS	-	expression tag	UNP Q8U2X0
D	477	HIS	-	expression tag	UNP Q8U2X0
D	478	HIS	-	expression tag	UNP Q8U2X0
D	479	HIS	-	expression tag	UNP Q8U2X0
D	480	HIS	-	expression tag	UNP Q8U2X0
D	481	HIS	-	expression tag	UNP Q8U2X0
D	482	HIS	-	expression tag	UNP Q8U2X0
D	483	HIS	-	expression tag	UNP Q8U2X0
D	484	HIS	-	expression tag	UNP Q8U2X0
D	485	HIS	-	expression tag	UNP Q8U2X0

- Molecule 2 is PENTAETHYLENE GLYCOL MONODECYL ETHER (CCD ID: CXE) (formula: C<sub>20</sub>H<sub>42</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 26 20 6	0	0
2	A	1	Total C O 26 20 6	0	0
2	A	1	Total C O 26 20 6	0	0
2	A	1	Total C O 20 16 4	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C O 20 16 4	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C O 14 12 2	0	0
2	A	1	Total C O 23 18 5	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 6 6	0	0
2	A	1	Total C O 20 16 4	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 7 7	0	0
2	A	1	Total C 5 5	0	0
2	B	1	Total C O 26 20 6	0	0
2	B	1	Total C O 20 16 4	0	0
2	B	1	Total C O 17 14 3	0	0
2	B	1	Total C O 11 10 1	0	0
2	B	1	Total C 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 17 14 3	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 7 7	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 9 9	0	0
2	C	1	Total C O 26 20 6	0	0
2	C	1	Total C O 26 20 6	0	0
2	C	1	Total C O 26 20 6	0	0
2	C	1	Total C O 26 20 6	0	0
2	C	1	Total C O 20 16 4	0	0
2	C	1	Total C O 15 13 2	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C 7 7	0	0
2	C	1	Total C O 17 14 3	0	0
2	C	1	Total C O 23 18 5	0	0
2	C	1	Total C 10 10	0	0
2	C	1	Total C O 16 10 6	0	0
2	C	1	Total C O 23 18 5	0	0
2	C	1	Total C O 17 14 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C 4 4	0	0
2	C	1	Total C 7 7	0	0
2	D	1	Total C O 11 10 1	0	0
2	D	1	Total C O 20 16 4	0	0
2	D	1	Total C O 14 12 2	0	0
2	D	1	Total C 10 10	0	0
2	D	1	Total C O 14 12 2	0	0
2	D	1	Total C O 11 10 1	0	0
2	D	1	Total C O 11 10 1	0	0
2	D	1	Total C 5 5	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0

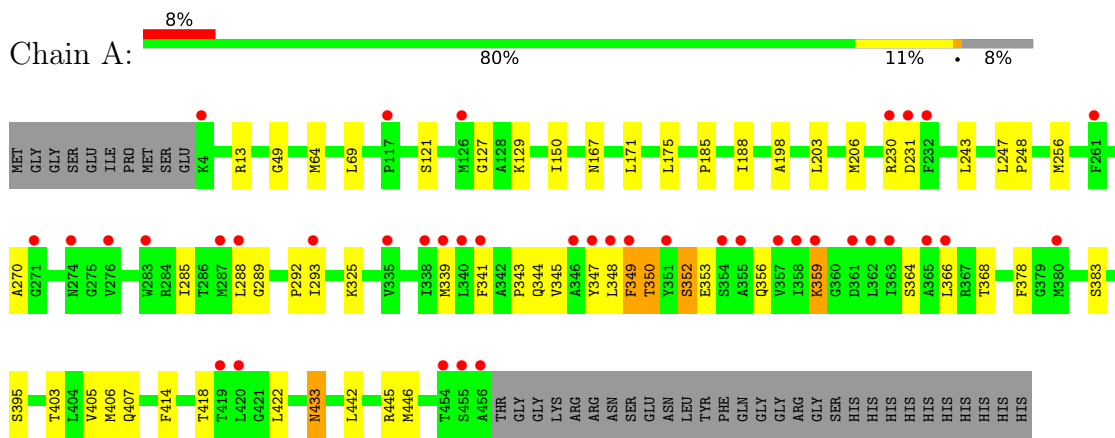
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	111	Total O 111 111	0	0
4	B	74	Total O 74 74	0	0
4	C	112	Total O 112 112	0	0
4	D	30	Total O 30 30	0	0

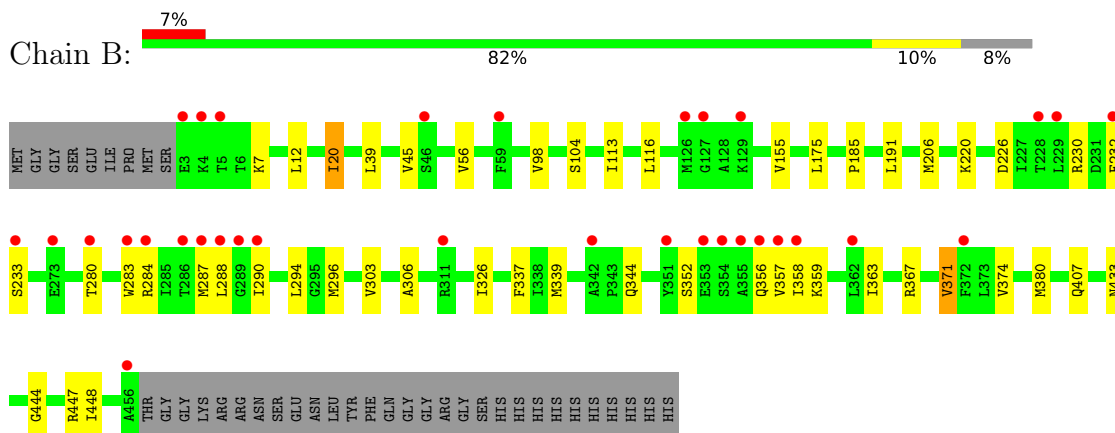
### 3 Residue-property plots [i](#)

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.

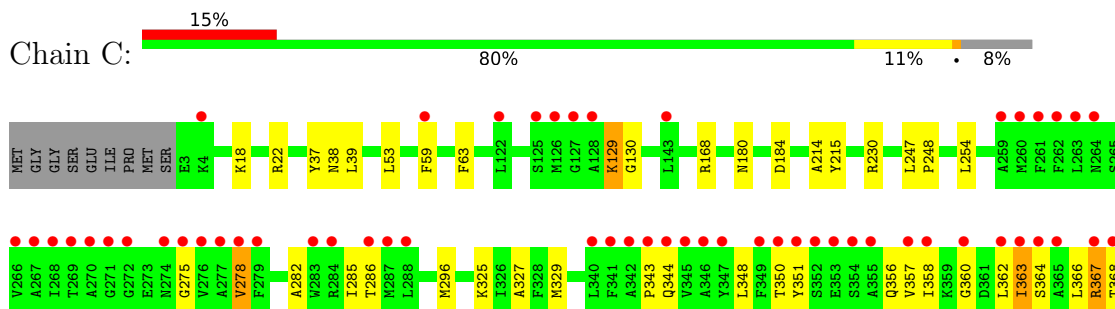
- Molecule 1: PF0708

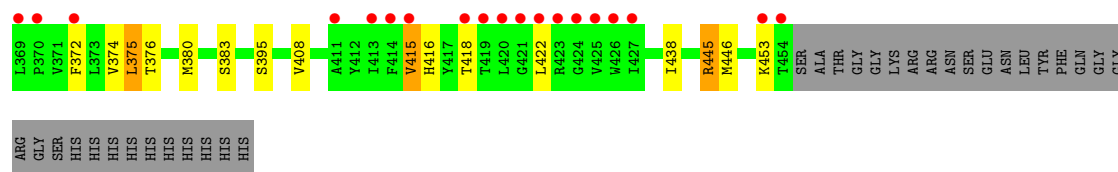


- Molecule 1: PF0708

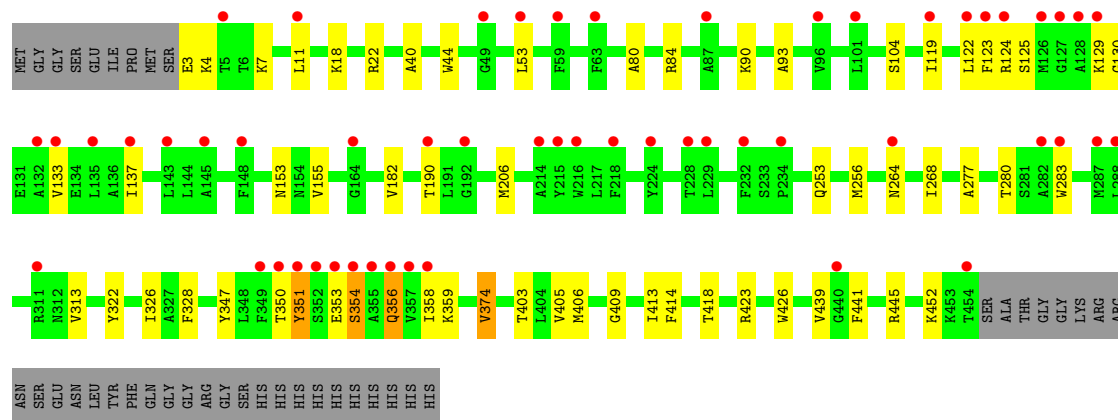
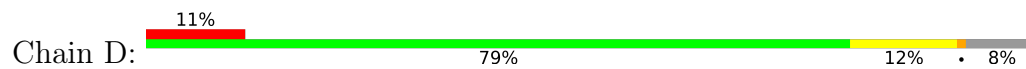


- Molecule 1: PF0708





- Molecule 1: PF0708



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	219.56Å 94.55Å 138.82Å 90.00° 126.47° 90.00°	Depositor
Resolution (Å)	45.24 – 2.35 45.24 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.24-2.35) 99.7 (45.24-2.35)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.203 , 0.231 0.199 , 0.228	Depositor DCC
$R_{free}$ test set	4737 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtrriage
Anisotropy	0.244	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.015 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CL, CXE

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	0.36	0/3476	0.82	4/4714 (0.1%)
1	B	0.33	0/3474	0.76	0/4712
1	C	0.36	0/3485	0.78	0/4725
1	D	0.33	0/3485	0.80	3/4725 (0.1%)
All	All	0.34	0/13920	0.79	7/18876 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	351	TYR	N-CA-C	9.27	121.32	111.03
1	A	231	ASP	N-CA-C	-8.03	102.96	114.12
1	D	354	SER	N-CA-C	6.57	119.05	109.07
1	A	49	GLY	CA-C-N	5.88	125.58	119.05
1	A	49	GLY	C-N-CA	5.88	125.58	119.05
1	D	130	GLY	N-CA-C	5.49	119.48	112.13
1	A	127	GLY	N-CA-C	-5.18	108.17	115.32

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3412	0	3601	36	0
1	B	3413	0	3594	31	0
1	C	3418	0	3610	44	0
1	D	3418	0	3610	36	0
2	A	246	0	420	20	0
2	B	144	0	253	11	0
2	C	273	0	450	24	0
2	D	96	0	174	8	0
3	A	2	0	0	1	0
4	A	111	0	0	4	0
4	B	74	0	0	1	0
4	C	112	0	0	0	0
4	D	30	0	0	1	0
All	All	14749	0	15712	166	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 6.

All (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLN:HG2	2:B:506:CXE:H091	1.59	0.82
1:C:445:ARG:HH11	1:C:445:ARG:HG2	1.51	0.76
1:A:349:PHE:HD2	1:A:349:PHE:H	1.37	0.72
2:B:501:CXE:H222	1:C:39:LEU:HD11	1.72	0.72
2:A:501:CXE:H062	2:A:515:CXE:H022	1.74	0.70
1:D:356:GLN:HE22	1:D:359:LYS:HD2	1.57	0.67
1:A:407:GLN:OE1	1:A:433:ASN:ND2	2.27	0.67
1:C:278:VAL:HG11	1:C:422:LEU:HD11	1.77	0.66
1:A:325:LYS:NZ	4:A:706:HOH:O	2.29	0.66
1:A:353:GLU:HB3	1:A:356:GLN:HE21	1.61	0.66
1:D:153:ASN:HD22	1:D:206:MET:HE3	1.60	0.66
1:A:175:LEU:HB2	2:A:506:CXE:H052	1.79	0.65
1:B:337:PHE:HZ	2:B:506:CXE:H032	1.62	0.64
1:C:348:LEU:HD11	2:C:513:CXE:H013	1.78	0.64
1:A:171:LEU:HD13	2:A:506:CXE:H091	1.80	0.63
2:A:503:CXE:H062	2:A:509:CXE:H032	1.82	0.61
1:C:445:ARG:HG2	1:C:445:ARG:NH1	2.15	0.61
1:D:414:PHE:O	1:D:418:THR:OG1	2.17	0.61
1:D:84:ARG:NH1	4:D:609:HOH:O	2.34	0.61
1:B:230:ARG:NH2	4:B:647:HOH:O	2.33	0.60
1:C:372:PHE:HA	1:C:375:LEU:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:NH2	4:A:609:HOH:O	2.30	0.59
2:A:502:CXE:H101	1:B:175:LEU:HB2	1.84	0.59
1:C:343:PRO:HB2	2:C:513:CXE:H132	1.83	0.59
1:A:348:LEU:O	1:A:352:SER:HB2	2.02	0.58
2:A:516:CXE:H061	1:D:190:THR:HA	1.85	0.58
1:C:357:VAL:HG13	1:C:358:ILE:HD12	1.85	0.58
1:B:339:MET:O	1:B:367:ARG:NE	2.34	0.57
1:C:275:GLY:HA2	1:C:278:VAL:HB	1.86	0.57
1:A:445:ARG:NH1	4:A:633:HOH:O	2.24	0.57
2:D:503:CXE:H071	2:D:505:CXE:H072	1.87	0.56
1:A:405:VAL:HG12	1:A:406:MET:HE2	1.88	0.56
1:C:356:GLN:O	1:C:360:GLY:N	2.33	0.56
1:B:45:VAL:HG11	1:B:56:VAL:HG21	1.87	0.56
1:B:339:MET:HE1	1:B:371:VAL:HG23	1.87	0.56
2:B:502:CXE:H021	2:C:505:CXE:H051	1.88	0.56
1:C:278:VAL:HG13	1:C:362:LEU:HD21	1.88	0.56
2:D:504:CXE:H082	2:D:505:CXE:H081	1.89	0.55
1:D:439:VAL:HG22	2:D:502:CXE:H051	1.88	0.55
2:A:506:CXE:H101	1:B:185:PRO:HB2	1.89	0.55
2:B:502:CXE:H072	2:C:505:CXE:H131	1.89	0.53
1:C:438:ILE:HD13	1:D:40:ALA:HB2	1.90	0.53
1:A:270:ALA:HB1	1:A:422:LEU:HA	1.90	0.53
1:A:185:PRO:HB2	2:A:502:CXE:H151	1.90	0.53
1:A:343:PRO:O	1:A:347:TYR:HB2	2.09	0.52
1:C:254:LEU:HB2	2:C:511:CXE:H061	1.92	0.52
1:B:352:SER:O	1:B:356:GLN:NE2	2.42	0.52
1:D:253:GLN:HA	1:D:256:MET:HE3	1.91	0.51
1:A:188:ILE:HD11	1:A:198:ALA:HB2	1.91	0.51
1:A:185:PRO:HG2	2:A:502:CXE:H131	1.93	0.51
1:C:358:ILE:O	1:C:362:LEU:HG	2.11	0.51
1:A:349:PHE:N	1:A:349:PHE:CD2	2.77	0.50
1:D:44:TRP:HZ3	2:D:507:CXE:H062	1.77	0.50
1:C:215:TYR:CD1	2:C:501:CXE:H132	2.46	0.50
1:D:123:PHE:HD2	1:D:137:ILE:HD13	1.77	0.49
1:A:64:MET:HB3	2:A:513:CXE:H101	1.94	0.49
1:C:329:MET:HE2	2:C:505:CXE:H081	1.95	0.49
1:A:344:GLN:N	1:A:344:GLN:OE1	2.45	0.49
2:C:505:CXE:H121	2:C:514:CXE:H013	1.94	0.49
1:C:383:SER:OG	1:C:395:SER:OG	2.29	0.49
1:B:287:MET:HA	1:B:290:ILE:HG23	1.95	0.48
1:C:129:LYS:HG2	1:C:130:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PHE:CZ	2:B:506:CXE:H032	2.46	0.48
2:A:504:CXE:H091	2:A:517:CXE:H021	1.96	0.48
1:B:20:ILE:HD12	1:B:303:VAL:HG21	1.95	0.48
1:D:133:VAL:O	1:D:137:ILE:HG12	2.14	0.48
2:A:506:CXE:H031	1:B:185:PRO:HG3	1.96	0.48
1:C:37:TYR:HE2	2:C:512:CXE:H181	1.78	0.47
2:C:513:CXE:H091	2:C:513:CXE:H062	1.68	0.47
1:A:230:ARG:NE	1:A:230:ARG:HA	2.28	0.47
1:D:44:TRP:CZ3	2:D:507:CXE:H062	2.49	0.47
1:B:206:MET:HA	1:B:206:MET:HE2	1.97	0.47
1:A:203:LEU:HA	1:A:206:MET:HE2	1.97	0.47
2:B:502:CXE:H092	2:C:505:CXE:H152	1.96	0.46
1:C:296:MET:HG3	1:C:327:ALA:HB2	1.97	0.46
1:D:277:ALA:HB3	1:D:358:ILE:HD13	1.97	0.46
1:A:341:PHE:O	1:A:345:VAL:HG23	2.15	0.46
1:A:350:THR:HG21	1:A:359:LYS:N	2.29	0.46
1:B:357:VAL:HG23	1:B:358:ILE:HG23	1.96	0.46
1:C:230:ARG:HA	2:C:502:CXE:H162	1.98	0.46
1:C:376:THR:HG22	1:C:380:MET:HG3	1.98	0.46
1:D:104:SER:HB3	1:D:155:VAL:HG21	1.95	0.46
3:A:518:CL:CL	4:A:652:HOH:O	2.58	0.46
1:B:113:ILE:HD11	2:C:503:CXE:H071	1.98	0.46
1:B:296:MET:HE1	1:B:326:ILE:HB	1.98	0.46
1:C:325:LYS:HG2	2:C:514:CXE:H032	1.98	0.46
1:C:374:VAL:HG11	1:D:182:VAL:HG13	1.97	0.46
1:A:353:GLU:HG2	1:A:356:GLN:HG3	1.98	0.46
1:A:256:MET:HG2	1:A:403:THR:HG21	1.98	0.45
1:C:362:LEU:O	1:C:366:LEU:HG	2.16	0.45
2:C:504:CXE:H212	2:C:504:CXE:H242	1.46	0.45
1:A:350:THR:HG21	1:A:359:LYS:HB3	1.99	0.45
1:B:407:GLN:OE1	1:B:433:ASN:ND2	2.46	0.45
1:A:69:LEU:HD21	2:A:513:CXE:H021	1.98	0.45
1:C:59:PHE:CZ	1:C:63:PHE:HB2	2.52	0.45
1:C:282:ALA:HA	1:C:285:ILE:HD12	1.99	0.45
1:A:378:PHE:CE2	2:A:507:CXE:H022	2.52	0.45
1:C:445:ARG:HH11	1:C:445:ARG:CG	2.25	0.44
1:B:294:LEU:HD23	1:B:380:MET:HE1	1.98	0.44
1:D:354:SER:HA	1:D:358:ILE:HD12	1.99	0.44
1:A:289:GLY:O	1:A:292:PRO:HD2	2.18	0.44
2:A:501:CXE:H082	2:A:515:CXE:H041	2.00	0.44
1:C:129:LYS:HB2	1:C:129:LYS:HE3	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:GLU:HA	1:D:90:LYS:HE3	1.99	0.44
1:D:7:LYS:HD2	1:D:7:LYS:HA	1.89	0.44
1:C:363:ILE:O	1:C:367:ARG:HD3	2.17	0.44
1:D:441:PHE:O	1:D:445:ARG:HG2	2.17	0.44
2:A:503:CXE:H191	2:B:506:CXE:H151	1.98	0.43
1:C:360:GLY:HA2	1:C:363:ILE:HG13	2.00	0.43
1:B:444:GLY:O	1:B:448:ILE:HG12	2.18	0.43
1:C:180:ASN:O	1:C:184:ASP:HB2	2.19	0.43
1:A:414:PHE:O	1:A:418:THR:OG1	2.22	0.43
1:C:344:GLN:H	1:C:344:GLN:CD	2.26	0.43
1:C:344:GLN:NE2	2:C:513:CXE:H212	2.33	0.43
1:D:405:VAL:HG12	1:D:406:MET:HE2	2.01	0.43
1:B:116:LEU:HD12	2:C:501:CXE:H121	1.99	0.43
1:D:328:PHE:HE1	1:D:374:VAL:HG13	1.84	0.43
2:A:506:CXE:H062	2:A:506:CXE:H092	1.75	0.42
2:C:504:CXE:H121	2:D:501:CXE:H081	2.01	0.42
1:A:442:LEU:O	1:A:446:MET:HB2	2.19	0.42
1:A:150:ILE:HG12	1:A:206:MET:SD	2.60	0.42
1:B:284:ARG:O	1:B:288:LEU:HD13	2.20	0.42
2:A:501:CXE:H062	2:A:515:CXE:C2	2.48	0.42
1:B:7:LYS:HB2	2:B:503:CXE:H151	2.00	0.42
1:C:380:MET:HE2	1:C:380:MET:HB3	1.82	0.42
1:D:80:ALA:O	1:D:84:ARG:HG2	2.19	0.42
1:D:313:VAL:HG11	1:D:452:LYS:HG3	2.00	0.42
1:A:129:LYS:HA	1:A:129:LYS:HD2	1.92	0.42
1:C:214:ALA:HB1	2:C:503:CXE:H181	2.01	0.42
1:C:247:LEU:HB3	1:C:248:PRO:HD3	2.02	0.42
1:C:278:VAL:HG22	1:C:362:LEU:HD21	2.02	0.42
1:D:423:ARG:HA	1:D:426:TRP:CD1	2.54	0.42
1:C:38:ASN:OD1	2:C:512:CXE:H161	2.20	0.42
1:B:280:THR:HA	1:B:283:TRP:NE1	2.35	0.41
1:B:280:THR:HA	1:B:283:TRP:CD1	2.55	0.41
2:C:501:CXE:H131	2:C:503:CXE:C12	2.50	0.41
1:D:347:TYR:CD1	2:D:501:CXE:H071	2.55	0.41
1:A:167:ASN:HD21	2:A:501:CXE:H252	1.85	0.41
1:B:447:ARG:HA	1:B:447:ARG:HD2	1.93	0.41
1:C:415:VAL:HG12	1:C:416:HIS:ND1	2.36	0.41
1:D:409:GLY:O	1:D:413:ILE:HG12	2.19	0.41
1:A:285:ILE:HD12	1:A:366:LEU:HD21	2.03	0.41
1:C:18:LYS:HE2	1:C:22:ARG:HG3	2.03	0.41
2:C:503:CXE:H162	2:C:503:CXE:H192	1.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:HB3	1:A:248:PRO:HD3	2.02	0.41
1:D:11:LEU:HD21	1:D:22[A]:ARG:HB2	2.02	0.41
1:B:12:LEU:HG	1:B:306:ALA:HB2	2.03	0.41
1:D:84:ARG:HB2	1:D:93:ALA:HB2	2.03	0.41
1:D:280:THR:HA	1:D:283:TRP:CD1	2.56	0.41
1:C:446:MET:SD	1:D:351:TYR:HB3	2.61	0.41
1:D:4:LYS:HD2	1:D:4:LYS:HA	1.69	0.41
1:D:18:LYS:HB2	1:D:18:LYS:HE3	1.81	0.41
1:D:256:MET:HG2	1:D:403:THR:HG21	2.02	0.41
1:D:356:GLN:NE2	1:D:359:LYS:HD2	2.30	0.41
1:B:104:SER:HB3	1:B:155:VAL:HG21	2.03	0.40
1:C:180:ASN:HD22	2:C:512:CXE:H222	1.86	0.40
2:A:501:CXE:H041	2:A:506:CXE:H011	2.03	0.40
1:C:325:LYS:HD3	2:D:507:CXE:H042	2.02	0.40
1:D:264:ASN:O	1:D:268:ILE:HG13	2.22	0.40
1:B:191:LEU:C	2:B:502:CXE:H102	2.46	0.40
1:B:359:LYS:NZ	1:B:363:ILE:HD11	2.37	0.40
2:B:506:CXE:H062	2:B:506:CXE:H092	1.75	0.40
2:C:506:CXE:H102	2:C:516:CXE:H042	2.04	0.40
1:A:383:SER:OG	1:A:395:SER:OG	2.38	0.40
1:B:98:VAL:HG11	1:B:232:PHE:HB2	2.03	0.40
1:D:322:TYR:CE2	1:D:326:ILE:HD11	2.56	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	452/492 (92%)	444 (98%)	8 (2%)	0	100	100
1	B	452/492 (92%)	446 (99%)	6 (1%)	0	100	100
1	C	452/492 (92%)	444 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	452/492 (92%)	445 (98%)	7 (2%)	0	100	100
All	All	1808/1968 (92%)	1779 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	358/389 (92%)	346 (97%)	12 (3%)	32	42
1	B	358/389 (92%)	351 (98%)	7 (2%)	48	61
1	C	359/389 (92%)	342 (95%)	17 (5%)	23	30
1	D	359/389 (92%)	349 (97%)	10 (3%)	38	50
All	All	1434/1556 (92%)	1388 (97%)	46 (3%)	34	44

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	243	LEU
1	A	288	LEU
1	A	293	ILE
1	A	339	MET
1	A	349	PHE
1	A	350	THR
1	A	352	SER
1	A	359	LYS
1	A	364	SER
1	A	368	THR
1	A	433	ASN
1	B	20	ILE
1	B	39	LEU
1	B	220	LYS
1	B	226	ASP

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Mol	Chain	Res	Type
1	B	233	SER
1	B	371	VAL
1	B	374	VAL
1	C	53	LEU
1	C	129	LYS
1	C	168	ARG
1	C	278	VAL
1	C	286	THR
1	C	350	THR
1	C	351	TYR
1	C	363	ILE
1	C	364	SER
1	C	367	ARG
1	C	368	THR
1	C	375	LEU
1	C	408	VAL
1	C	415	VAL
1	C	418	THR
1	C	445	ARG
1	C	453	LYS
1	D	53	LEU
1	D	119	ILE
1	D	122	LEU
1	D	124	ARG
1	D	125	SER
1	D	129	LYS
1	D	350	THR
1	D	353	GLU
1	D	356	GLN
1	D	374	VAL

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	34	GLN
1	A	356	GLN
1	A	407	GLN
1	A	433	ASN
1	B	167	ASN
1	B	407	GLN
1	B	433	ASN
1	C	180	ASN

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Mol	Chain	Res	Type
1	C	407	GLN
1	D	34	GLN
1	D	38	ASN
1	D	356	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 55 ligands modelled in this entry, 2 are monoatomic - leaving 53 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CXE	D	505	-	13,13,25	0.27	0	12,12,24	0.50	0
2	CXE	D	501	-	10,10,25	0.20	0	9,9,24	0.58	0
2	CXE	C	514	-	16,16,25	0.34	0	15,15,24	0.46	0
2	CXE	A	511	-	9,9,25	0.22	0	8,8,24	0.57	0
2	CXE	A	506	-	19,19,25	0.31	0	18,18,24	0.55	0
2	CXE	B	510	-	5,5,25	0.23	0	4,4,24	0.43	0
2	CXE	C	503	-	25,25,25	0.39	0	24,24,24	0.60	0
2	CXE	A	509	-	22,22,25	0.38	0	21,21,24	0.40	0
2	CXE	B	503	-	16,16,25	0.33	0	15,15,24	0.59	0
2	CXE	A	505	-	9,9,25	0.17	0	8,8,24	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CXE	A	513	-	19,19,25	0.32	0	18,18,24	0.52	0
2	CXE	B	506	-	16,16,25	0.36	0	15,15,24	0.51	0
2	CXE	D	508	-	4,4,25	0.24	0	3,3,24	0.40	0
2	CXE	B	512	-	8,8,25	0.25	0	7,7,24	0.46	0
2	CXE	A	502	-	25,25,25	0.40	0	24,24,24	0.42	0
2	CXE	B	511	-	5,5,25	0.26	0	4,4,24	0.43	0
2	CXE	C	511	-	9,9,25	0.23	0	8,8,24	0.57	0
2	CXE	C	506	-	14,14,25	0.32	0	13,13,24	0.54	0
2	CXE	C	501	-	25,25,25	0.41	0	24,24,24	0.43	0
2	CXE	B	501	-	25,25,25	0.39	0	24,24,24	0.44	0
2	CXE	C	507	-	9,9,25	0.25	0	8,8,24	0.49	0
2	CXE	D	507	-	10,10,25	0.23	0	9,9,24	0.51	0
2	CXE	A	504	-	19,19,25	0.31	0	18,18,24	0.59	0
2	CXE	A	503	-	25,25,25	0.33	0	24,24,24	0.68	0
2	CXE	C	516	-	6,6,25	0.26	0	5,5,24	0.50	0
2	CXE	A	517	-	4,4,25	0.22	0	3,3,24	0.54	0
2	CXE	C	509	-	16,16,25	0.37	0	15,15,24	0.56	0
2	CXE	D	506	-	10,10,25	0.24	0	9,9,24	0.50	0
2	CXE	B	504	-	10,10,25	0.24	0	9,9,24	0.50	0
2	CXE	C	512	-	15,15,25	0.45	0	14,14,24	0.43	0
2	CXE	A	507	-	6,6,25	0.24	0	5,5,24	0.42	0
2	CXE	A	510	-	9,9,25	0.23	0	8,8,24	0.55	0
2	CXE	D	502	-	19,19,25	0.29	0	18,18,24	0.58	0
2	CXE	A	516	-	6,6,25	0.20	0	5,5,24	0.64	0
2	CXE	C	502	-	25,25,25	0.37	0	24,24,24	0.57	0
2	CXE	C	504	-	25,25,25	0.40	0	24,24,24	0.48	0
2	CXE	C	515	-	3,3,25	0.33	0	2,2,24	0.63	0
2	CXE	A	514	-	8,8,25	0.23	0	7,7,24	0.52	0
2	CXE	B	508	-	6,6,25	0.25	0	5,5,24	0.42	0
2	CXE	C	508	-	6,6,25	0.23	0	5,5,24	0.54	0
2	CXE	A	501	-	25,25,25	0.40	0	24,24,24	0.51	0
2	CXE	B	502	-	19,19,25	0.42	0	18,18,24	0.47	0
2	CXE	D	503	-	13,13,25	0.30	0	12,12,24	0.49	0
2	CXE	B	507	-	8,8,25	0.21	0	7,7,24	0.60	0
2	CXE	C	513	-	22,22,25	0.35	0	21,21,24	0.65	0
2	CXE	A	512	-	5,5,25	0.25	0	4,4,24	0.42	0
2	CXE	C	510	-	22,22,25	0.37	0	21,21,24	0.50	0
2	CXE	D	504	-	9,9,25	0.21	0	8,8,24	0.63	0
2	CXE	A	508	-	13,13,25	0.29	0	12,12,24	0.52	0
2	CXE	B	509	-	5,5,25	0.25	0	4,4,24	0.37	0
2	CXE	A	515	-	6,6,25	0.24	0	5,5,24	0.43	0
2	CXE	C	505	-	19,19,25	0.38	0	18,18,24	0.74	0
2	CXE	B	505	-	9,9,25	0.23	0	8,8,24	0.55	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	CXE	D	505	-	-	3/11/11/23	-
2	CXE	D	501	-	-	2/8/8/23	-
2	CXE	C	514	-	-	3/14/14/23	-
2	CXE	A	511	-	-	2/7/7/23	-
2	CXE	A	506	-	-	8/17/17/23	-
2	CXE	B	510	-	-	1/3/3/23	-
2	CXE	C	503	-	-	12/23/23/23	-
2	CXE	A	509	-	-	3/20/20/23	-
2	CXE	B	503	-	-	10/14/14/23	-
2	CXE	A	505	-	-	3/7/7/23	-
2	CXE	A	513	-	-	7/17/17/23	-
2	CXE	B	506	-	-	6/14/14/23	-
2	CXE	D	508	-	-	0/2/2/23	-
2	CXE	B	512	-	-	4/6/6/23	-
2	CXE	A	502	-	-	3/23/23/23	-
2	CXE	B	511	-	-	2/3/3/23	-
2	CXE	C	511	-	-	0/7/7/23	-
2	CXE	C	506	-	-	9/12/12/23	-
2	CXE	C	501	-	-	10/23/23/23	-
2	CXE	B	501	-	-	1/23/23/23	-
2	CXE	C	507	-	-	3/7/7/23	-
2	CXE	D	507	-	-	4/8/8/23	-
2	CXE	A	504	-	-	8/17/17/23	-
2	CXE	A	503	-	-	10/23/23/23	-
2	CXE	C	516	-	-	3/4/4/23	-
2	CXE	A	517	-	-	2/2/2/23	-
2	CXE	C	509	-	-	8/14/14/23	-
2	CXE	D	506	-	-	7/8/8/23	-
2	CXE	B	504	-	-	0/8/8/23	-
2	CXE	C	512	-	-	8/13/13/23	-
2	CXE	A	507	-	-	2/4/4/23	-
2	CXE	A	510	-	-	3/7/7/23	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CXE	D	502	-	-	11/17/17/23	-
2	CXE	A	516	-	-	2/4/4/23	-
2	CXE	C	502	-	-	13/23/23/23	-
2	CXE	C	504	-	-	12/23/23/23	-
2	CXE	C	515	-	-	1/1/1/23	-
2	CXE	A	514	-	-	3/6/6/23	-
2	CXE	B	508	-	-	2/4/4/23	-
2	CXE	C	508	-	-	1/4/4/23	-
2	CXE	A	501	-	-	7/23/23/23	-
2	CXE	B	502	-	-	6/17/17/23	-
2	CXE	D	503	-	-	7/11/11/23	-
2	CXE	B	507	-	-	3/6/6/23	-
2	CXE	C	513	-	-	12/20/20/23	-
2	CXE	A	512	-	-	0/3/3/23	-
2	CXE	C	510	-	-	7/20/20/23	-
2	CXE	D	504	-	-	2/7/7/23	-
2	CXE	A	508	-	-	9/11/11/23	-
2	CXE	B	509	-	-	1/3/3/23	-
2	CXE	A	515	-	-	2/4/4/23	-
2	CXE	C	505	-	-	9/17/17/23	-
2	CXE	B	505	-	-	0/7/7/23	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (257) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	504	CXE	C16-C15-O14-C13
2	C	503	CXE	C19-C18-O17-C16
2	A	513	CXE	O11-C12-C13-O14
2	C	513	CXE	O11-C12-C13-O14
2	D	502	CXE	O11-C12-C13-O14
2	A	501	CXE	O11-C12-C13-O14
2	A	503	CXE	O14-C15-C16-O17
2	C	502	CXE	O11-C12-C13-O14
2	B	506	CXE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	C	502	CXE	C4-C5-C6-C7
2	C	506	CXE	C9-C10-O11-C12
2	C	504	CXE	O23-C24-C25-O26
2	C	513	CXE	C6-C7-C8-C9
2	A	508	CXE	C6-C7-C8-C9
2	A	502	CXE	O11-C12-C13-O14
2	C	502	CXE	O17-C18-C19-O20
2	C	503	CXE	O17-C18-C19-O20
2	C	504	CXE	C21-C22-O23-C24
2	C	506	CXE	O11-C10-C9-C8
2	C	504	CXE	O20-C21-C22-O23
2	C	504	CXE	C3-C4-C5-C6
2	B	506	CXE	O11-C12-C13-O14
2	A	506	CXE	O11-C10-C9-C8
2	A	508	CXE	O11-C10-C9-C8
2	A	504	CXE	O17-C18-C19-O20
2	A	508	CXE	O11-C12-C13-O14
2	A	503	CXE	O11-C12-C13-O14
2	B	502	CXE	O11-C12-C13-O14
2	A	504	CXE	C4-C5-C6-C7
2	D	502	CXE	O11-C10-C9-C8
2	C	509	CXE	O14-C15-C16-O17
2	C	502	CXE	O14-C15-C16-O17
2	A	507	CXE	C3-C4-C5-C6
2	B	512	CXE	C4-C5-C6-C7
2	C	514	CXE	C5-C6-C7-C8
2	D	501	CXE	C6-C7-C8-C9
2	C	507	CXE	C5-C6-C7-C8
2	C	513	CXE	C5-C6-C7-C8
2	D	502	CXE	C2-C3-C4-C5
2	D	506	CXE	C5-C6-C7-C8
2	C	506	CXE	C3-C4-C5-C6
2	B	503	CXE	O11-C12-C13-O14
2	C	502	CXE	C7-C8-C9-C10
2	C	506	CXE	C4-C5-C6-C7
2	C	501	CXE	O11-C12-C13-O14
2	C	504	CXE	C19-C18-O17-C16
2	D	502	CXE	O14-C15-C16-O17
2	A	503	CXE	C3-C4-C5-C6
2	C	504	CXE	C5-C6-C7-C8
2	D	502	CXE	C5-C6-C7-C8
2	C	514	CXE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	A	506	CXE	O17-C18-C19-O20
2	C	513	CXE	O20-C21-C22-O23
2	D	505	CXE	O11-C12-C13-O14
2	A	506	CXE	C7-C8-C9-C10
2	A	511	CXE	C4-C5-C6-C7
2	D	503	CXE	C3-C4-C5-C6
2	A	504	CXE	O11-C12-C13-O14
2	B	503	CXE	C6-C7-C8-C9
2	B	512	CXE	C5-C6-C7-C8
2	A	504	CXE	C7-C8-C9-C10
2	C	516	CXE	C2-C3-C4-C5
2	D	506	CXE	C6-C7-C8-C9
2	C	510	CXE	O11-C10-C9-C8
2	A	510	CXE	C6-C7-C8-C9
2	D	502	CXE	C4-C5-C6-C7
2	C	505	CXE	C4-C5-C6-C7
2	C	505	CXE	O17-C18-C19-O20
2	C	512	CXE	O23-C24-C25-O26
2	A	510	CXE	C2-C3-C4-C5
2	B	507	CXE	C2-C3-C4-C5
2	B	508	CXE	C2-C3-C4-C5
2	A	510	CXE	C5-C6-C7-C8
2	D	503	CXE	C7-C8-C9-C10
2	B	503	CXE	C2-C3-C4-C5
2	A	503	CXE	C7-C8-C9-C10
2	C	507	CXE	C4-C5-C6-C7
2	A	514	CXE	C2-C3-C4-C5
2	C	505	CXE	C5-C6-C7-C8
2	C	506	CXE	C5-C6-C7-C8
2	A	509	CXE	C3-C4-C5-C6
2	C	503	CXE	C5-C6-C7-C8
2	D	502	CXE	C3-C4-C5-C6
2	A	513	CXE	O17-C18-C19-O20
2	C	502	CXE	O23-C24-C25-O26
2	A	513	CXE	O14-C15-C16-O17
2	C	506	CXE	O11-C12-C13-O14
2	C	502	CXE	C2-C3-C4-C5
2	C	509	CXE	C2-C3-C4-C5
2	C	506	CXE	C6-C7-C8-C9
2	A	504	CXE	O14-C15-C16-O17
2	C	503	CXE	O20-C21-C22-O23
2	C	514	CXE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	A	501	CXE	C5-C6-C7-C8
2	A	516	CXE	C2-C3-C4-C5
2	A	508	CXE	C5-C6-C7-C8
2	C	509	CXE	C6-C7-C8-C9
2	B	503	CXE	C9-C10-O11-C12
2	B	502	CXE	C3-C4-C5-C6
2	D	501	CXE	C4-C5-C6-C7
2	A	514	CXE	C6-C7-C8-C9
2	C	513	CXE	C4-C5-C6-C7
2	A	508	CXE	C2-C3-C4-C5
2	B	502	CXE	C2-C3-C4-C5
2	B	503	CXE	C7-C8-C9-C10
2	D	506	CXE	C2-C3-C4-C5
2	C	507	CXE	C1-C2-C3-C4
2	B	511	CXE	C2-C3-C4-C5
2	A	517	CXE	C2-C3-C4-C5
2	A	506	CXE	C1-C2-C3-C4
2	A	514	CXE	C1-C2-C3-C4
2	A	506	CXE	C6-C7-C8-C9
2	A	517	CXE	C1-C2-C3-C4
2	B	511	CXE	C3-C4-C5-C6
2	C	513	CXE	O14-C15-C16-O17
2	A	505	CXE	C6-C7-C8-C9
2	B	503	CXE	C3-C4-C5-C6
2	A	509	CXE	C2-C3-C4-C5
2	C	505	CXE	C3-C4-C5-C6
2	B	512	CXE	C2-C3-C4-C5
2	D	507	CXE	C4-C5-C6-C7
2	D	506	CXE	C7-C8-C9-C10
2	C	503	CXE	O11-C12-C13-O14
2	C	501	CXE	O17-C18-C19-O20
2	C	504	CXE	O17-C18-C19-O20
2	C	505	CXE	O11-C10-C9-C8
2	C	506	CXE	C7-C8-C9-C10
2	C	516	CXE	C4-C5-C6-C7
2	B	512	CXE	C1-C2-C3-C4
2	A	511	CXE	C3-C4-C5-C6
2	C	501	CXE	C21-C22-O23-C24
2	D	502	CXE	C19-C18-O17-C16
2	C	504	CXE	C6-C7-C8-C9
2	A	515	CXE	C1-C2-C3-C4
2	A	513	CXE	C13-C12-O11-C10

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Mol	Chain	Res	Type	Atoms
2	C	501	CXE	C22-C21-O20-C19
2	C	505	CXE	C12-C13-O14-C15
2	C	510	CXE	C12-C13-O14-C15
2	A	503	CXE	C22-C21-O20-C19
2	C	504	CXE	C18-C19-O20-C21
2	C	510	CXE	C13-C12-O11-C10
2	C	512	CXE	C16-C15-O14-C13
2	D	507	CXE	C7-C8-C9-C10
2	A	508	CXE	C4-C5-C6-C7
2	A	504	CXE	C13-C12-O11-C10
2	C	513	CXE	C16-C15-O14-C13
2	C	513	CXE	C22-C21-O20-C19
2	A	501	CXE	C1-C2-C3-C4
2	B	508	CXE	C4-C5-C6-C7
2	B	509	CXE	C3-C4-C5-C6
2	C	503	CXE	O23-C24-C25-O26
2	A	503	CXE	C19-C18-O17-C16
2	A	508	CXE	C7-C8-C9-C10
2	C	501	CXE	C12-C13-O14-C15
2	C	516	CXE	C3-C4-C5-C6
2	B	502	CXE	C5-C6-C7-C8
2	A	503	CXE	C25-C24-O23-C22
2	B	502	CXE	O11-C10-C9-C8
2	D	502	CXE	O17-C18-C19-O20
2	C	513	CXE	C2-C3-C4-C5
2	D	503	CXE	C2-C3-C4-C5
2	A	505	CXE	C1-C2-C3-C4
2	C	502	CXE	C9-C10-O11-C12
2	B	507	CXE	C3-C4-C5-C6
2	C	509	CXE	C9-C10-O11-C12
2	D	502	CXE	C9-C10-O11-C12
2	A	508	CXE	C3-C4-C5-C6
2	D	503	CXE	C6-C7-C8-C9
2	C	503	CXE	C21-C22-O23-C24
2	A	501	CXE	O11-C10-C9-C8
2	A	513	CXE	C15-C16-O17-C18
2	C	503	CXE	C13-C12-O11-C10
2	D	504	CXE	C6-C7-C8-C9
2	A	501	CXE	C9-C10-O11-C12
2	D	506	CXE	C4-C5-C6-C7
2	D	503	CXE	O11-C10-C9-C8
2	A	504	CXE	C12-C13-O14-C15

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Mol	Chain	Res	Type	Atoms
2	D	505	CXE	C9-C10-O11-C12
2	C	502	CXE	C12-C13-O14-C15
2	C	509	CXE	C16-C15-O14-C13
2	C	512	CXE	C18-C19-O20-C21
2	C	505	CXE	O14-C15-C16-O17
2	C	513	CXE	C13-C12-O11-C10
2	A	509	CXE	C5-C6-C7-C8
2	C	509	CXE	C13-C12-O11-C10
2	D	507	CXE	C5-C6-C7-C8
2	A	508	CXE	C9-C10-O11-C12
2	C	506	CXE	C2-C3-C4-C5
2	A	501	CXE	O14-C15-C16-O17
2	B	506	CXE	C13-C12-O11-C10
2	D	502	CXE	C7-C8-C9-C10
2	C	501	CXE	O20-C21-C22-O23
2	A	506	CXE	O14-C15-C16-O17
2	A	506	CXE	C9-C10-O11-C12
2	C	501	CXE	C19-C18-O17-C16
2	C	512	CXE	C21-C22-O23-C24
2	B	507	CXE	C5-C6-C7-C8
2	C	501	CXE	O11-C10-C9-C8
2	D	505	CXE	C7-C8-C9-C10
2	B	502	CXE	C12-C13-O14-C15
2	B	503	CXE	C5-C6-C7-C8
2	B	506	CXE	C3-C4-C5-C6
2	C	512	CXE	O14-C15-C16-O17
2	B	503	CXE	C12-C13-O14-C15
2	A	507	CXE	C4-C5-C6-C7
2	C	510	CXE	C16-C15-O14-C13
2	C	503	CXE	C25-C24-O23-C22
2	A	503	CXE	C15-C16-O17-C18
2	B	506	CXE	C16-C15-O14-C13
2	C	509	CXE	C4-C5-C6-C7
2	B	510	CXE	C2-C3-C4-C5
2	A	501	CXE	C21-C22-O23-C24
2	D	504	CXE	C2-C3-C4-C5
2	C	503	CXE	C18-C19-O20-C21
2	C	512	CXE	C22-C21-O20-C19
2	C	513	CXE	C15-C16-O17-C18
2	C	504	CXE	C15-C16-O17-C18
2	A	513	CXE	C1-C2-C3-C4
2	C	502	CXE	C15-C16-O17-C18

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Mol	Chain	Res	Type	Atoms
2	B	501	CXE	C9-C10-O11-C12
2	B	503	CXE	C13-C12-O11-C10
2	A	502	CXE	O14-C15-C16-O17
2	C	503	CXE	C9-C10-O11-C12
2	C	502	CXE	C6-C7-C8-C9
2	C	502	CXE	O20-C21-C22-O23
2	C	510	CXE	C4-C5-C6-C7
2	D	503	CXE	C1-C2-C3-C4
2	B	503	CXE	C16-C15-O14-C13
2	A	502	CXE	C4-C5-C6-C7
2	C	501	CXE	C13-C12-O11-C10
2	C	509	CXE	C12-C13-O14-C15
2	A	505	CXE	C5-C6-C7-C8
2	A	506	CXE	O11-C12-C13-O14
2	C	503	CXE	O14-C15-C16-O17
2	A	515	CXE	C4-C5-C6-C7
2	C	513	CXE	C18-C19-O20-C21
2	C	501	CXE	O14-C15-C16-O17
2	C	505	CXE	O11-C12-C13-O14
2	C	510	CXE	O14-C15-C16-O17
2	A	516	CXE	C4-C5-C6-C7
2	A	503	CXE	C16-C15-O14-C13
2	D	503	CXE	O11-C12-C13-O14
2	C	512	CXE	O17-C18-C19-O20
2	B	506	CXE	O14-C15-C16-O17
2	C	508	CXE	C4-C5-C6-C7
2	D	507	CXE	C2-C3-C4-C5
2	A	503	CXE	O17-C18-C19-O20
2	D	506	CXE	C3-C4-C5-C6
2	C	510	CXE	O11-C12-C13-O14
2	C	505	CXE	C6-C7-C8-C9
2	A	513	CXE	C12-C13-O14-C15
2	C	515	CXE	C1-C2-C3-C4
2	C	502	CXE	C13-C12-O11-C10
2	C	504	CXE	O14-C15-C16-O17
2	D	506	CXE	O11-C10-C9-C8
2	A	504	CXE	C5-C6-C7-C8
2	C	512	CXE	C19-C18-O17-C16

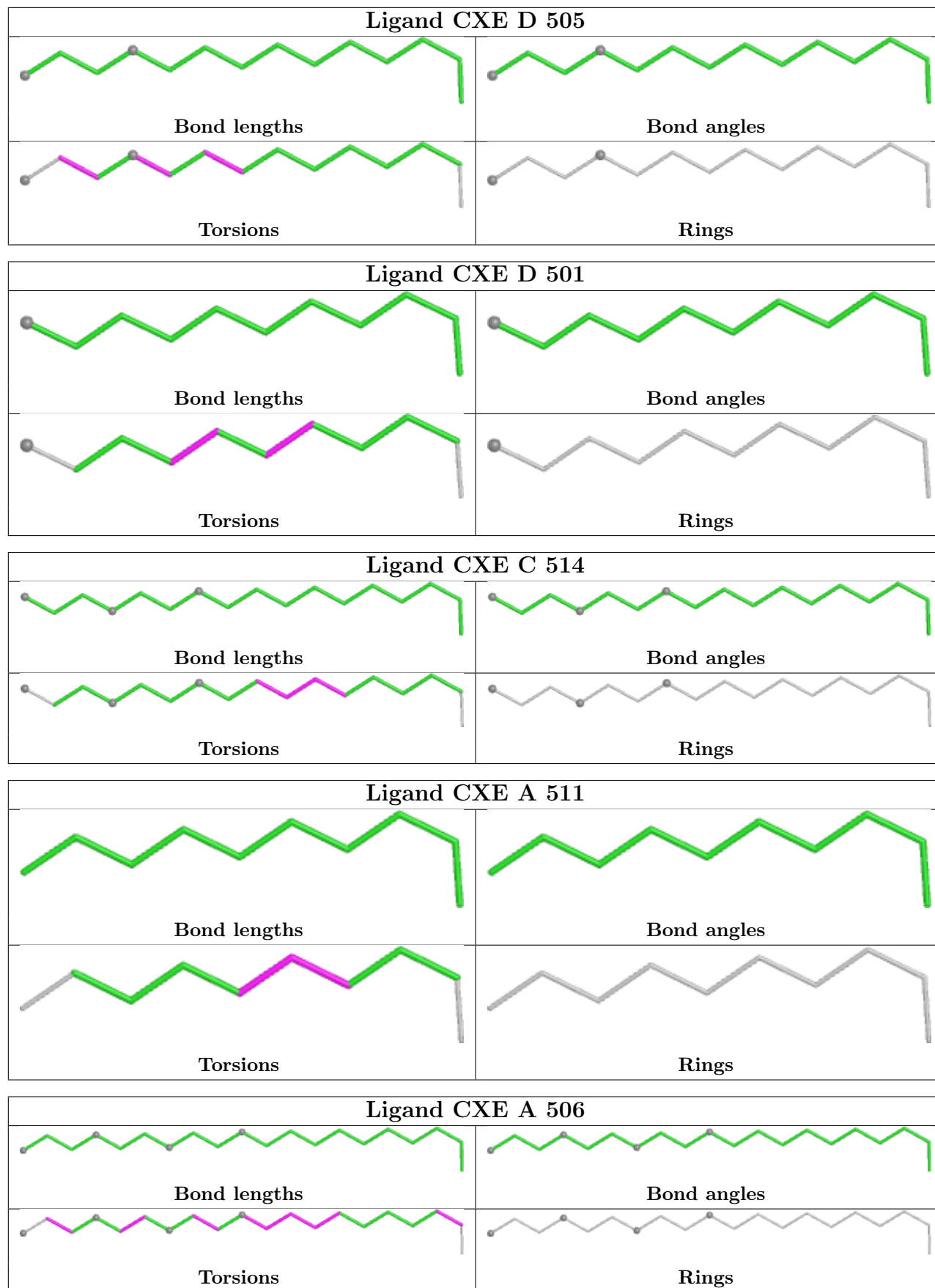
There are no ring outliers.

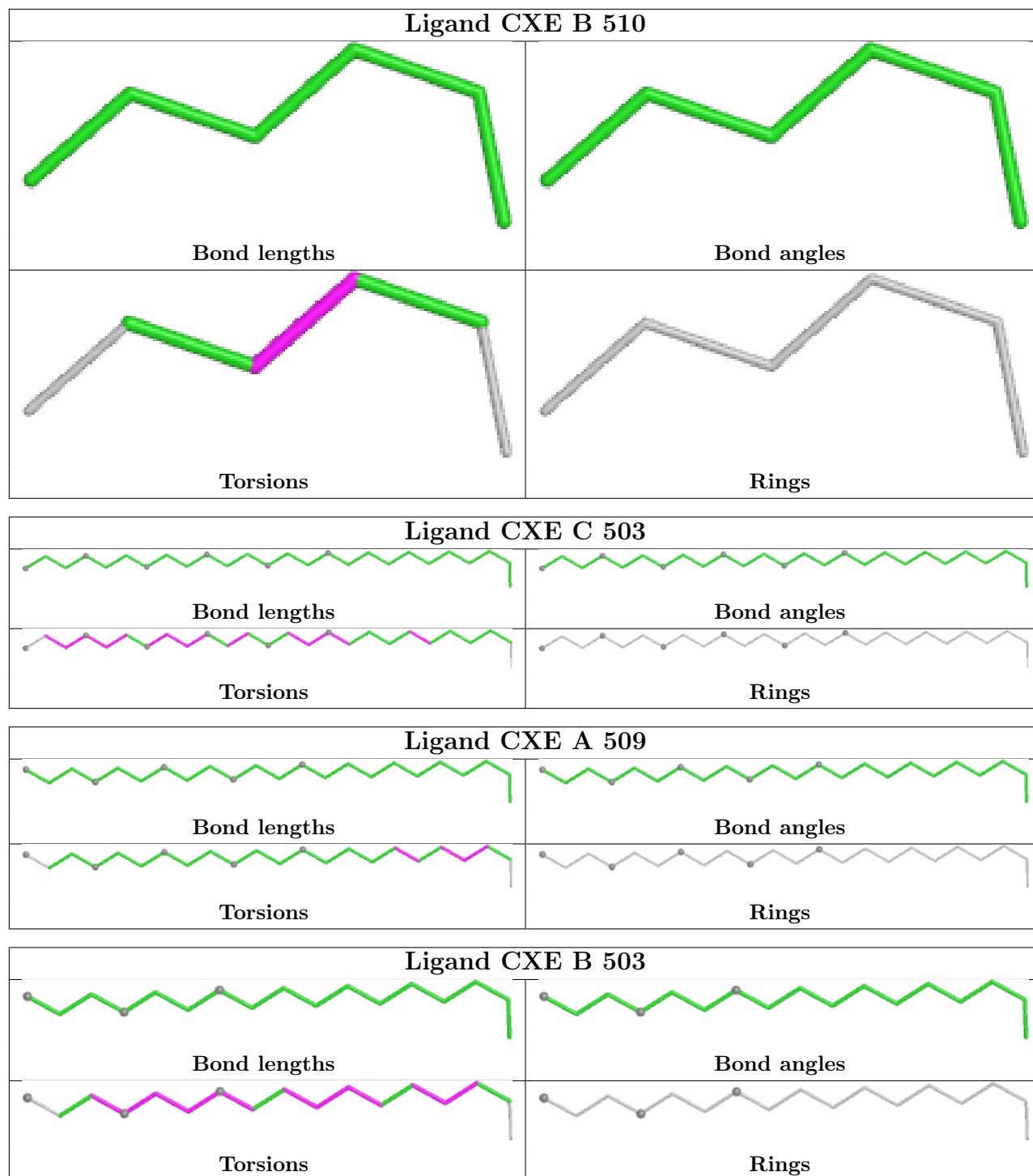
32 monomers are involved in 58 short contacts:

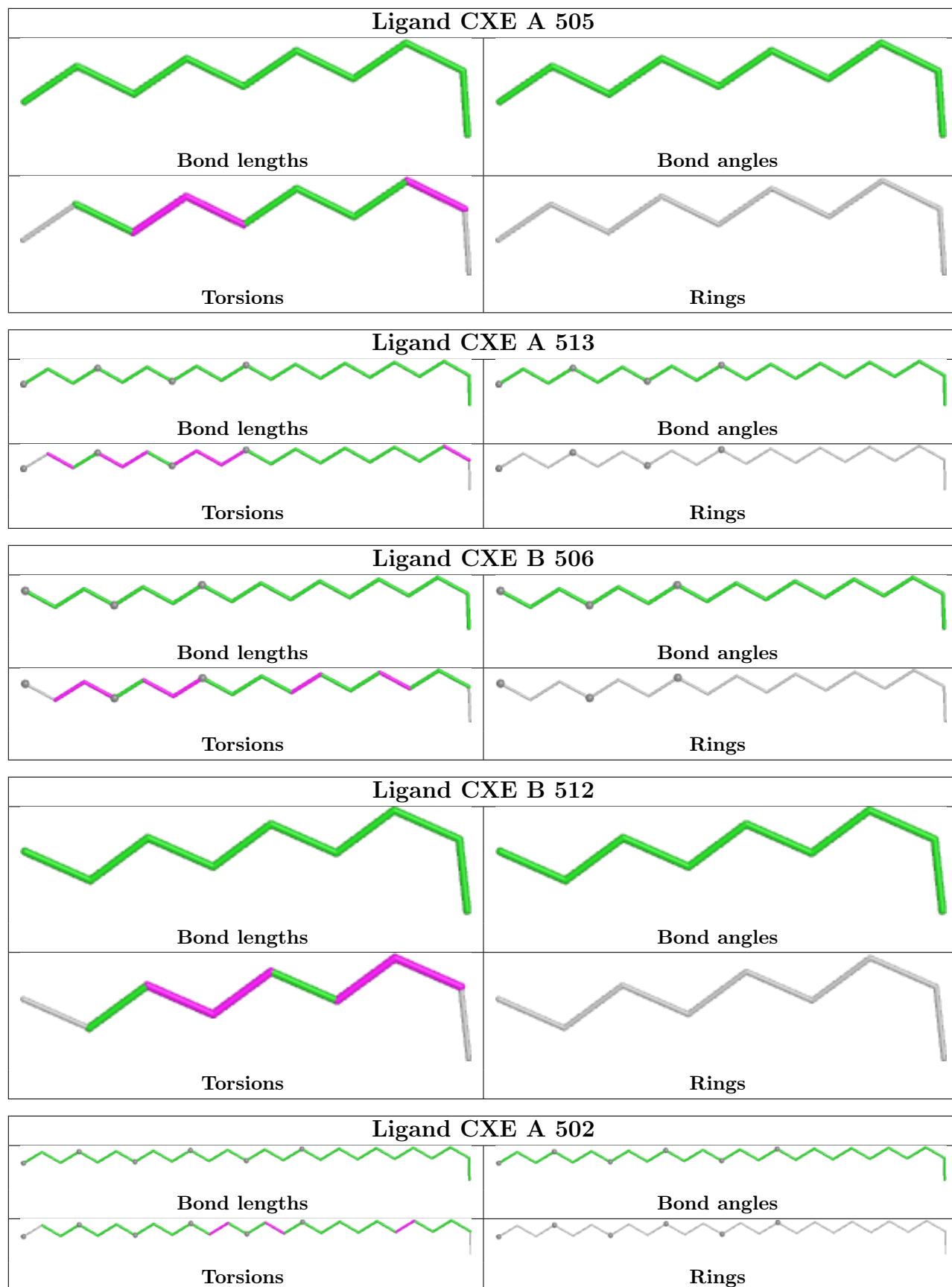
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	505	CXE	2	0
2	D	501	CXE	2	0
2	C	514	CXE	2	0
2	A	506	CXE	6	0
2	C	503	CXE	4	0
2	A	509	CXE	1	0
2	B	503	CXE	1	0
2	A	513	CXE	2	0
2	B	506	CXE	5	0
2	A	502	CXE	3	0
2	C	511	CXE	1	0
2	C	506	CXE	1	0
2	C	501	CXE	3	0
2	B	501	CXE	1	0
2	D	507	CXE	3	0
2	A	504	CXE	1	0
2	A	503	CXE	2	0
2	C	516	CXE	1	0
2	A	517	CXE	1	0
2	C	512	CXE	3	0
2	A	507	CXE	1	0
2	D	502	CXE	1	0
2	A	516	CXE	1	0
2	C	502	CXE	1	0
2	C	504	CXE	2	0
2	A	501	CXE	5	0
2	B	502	CXE	4	0
2	D	503	CXE	1	0
2	C	513	CXE	4	0
2	D	504	CXE	1	0
2	A	515	CXE	3	0
2	C	505	CXE	5	0

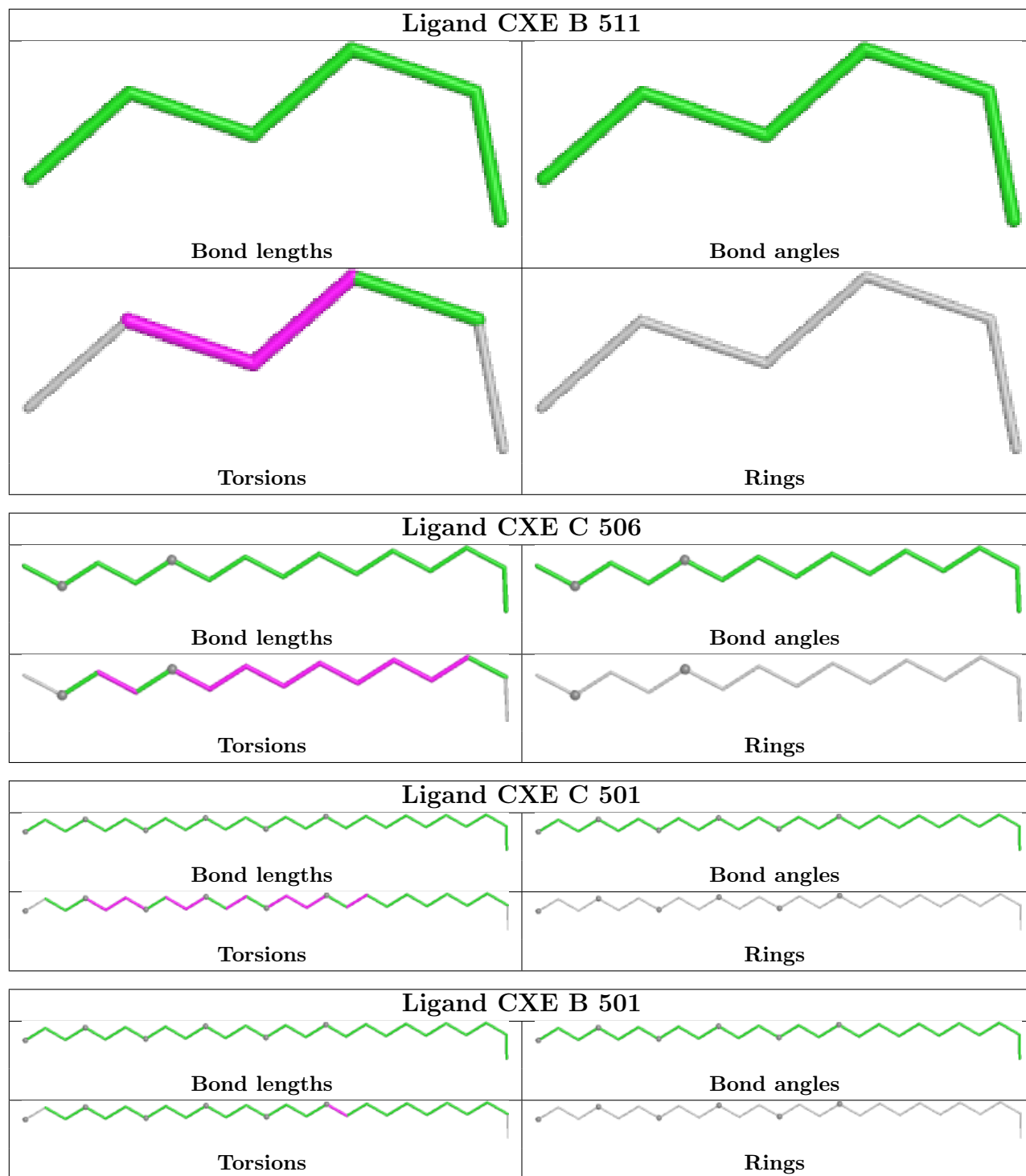
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

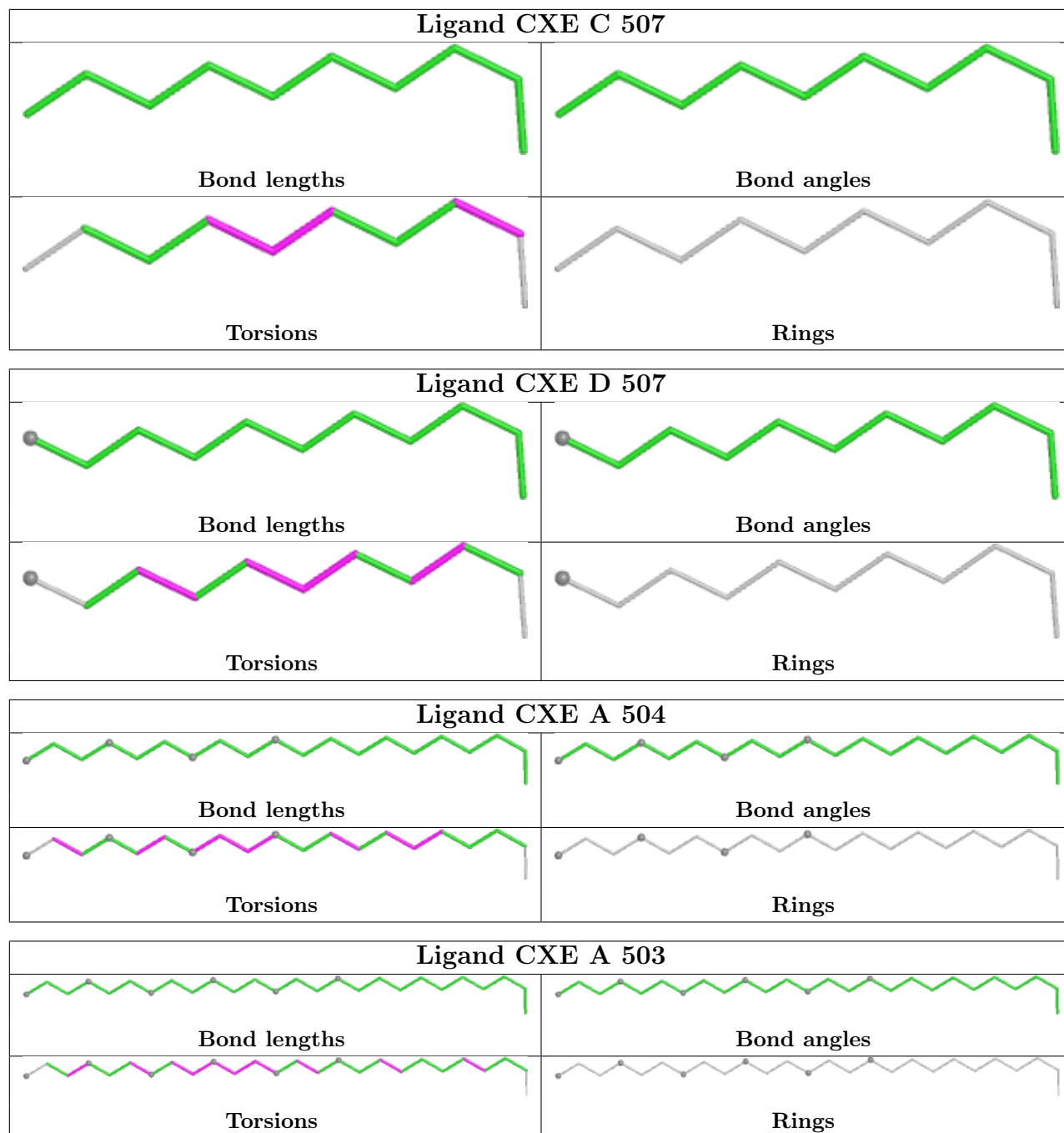
equivalents in the CSD to analyse the geometry.

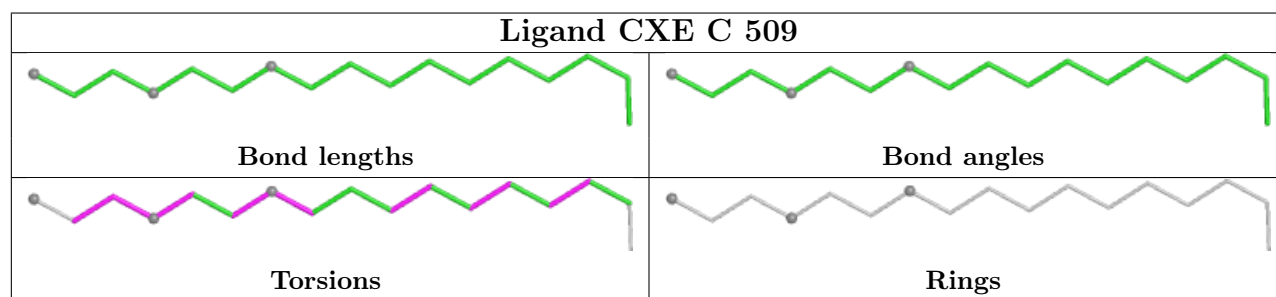
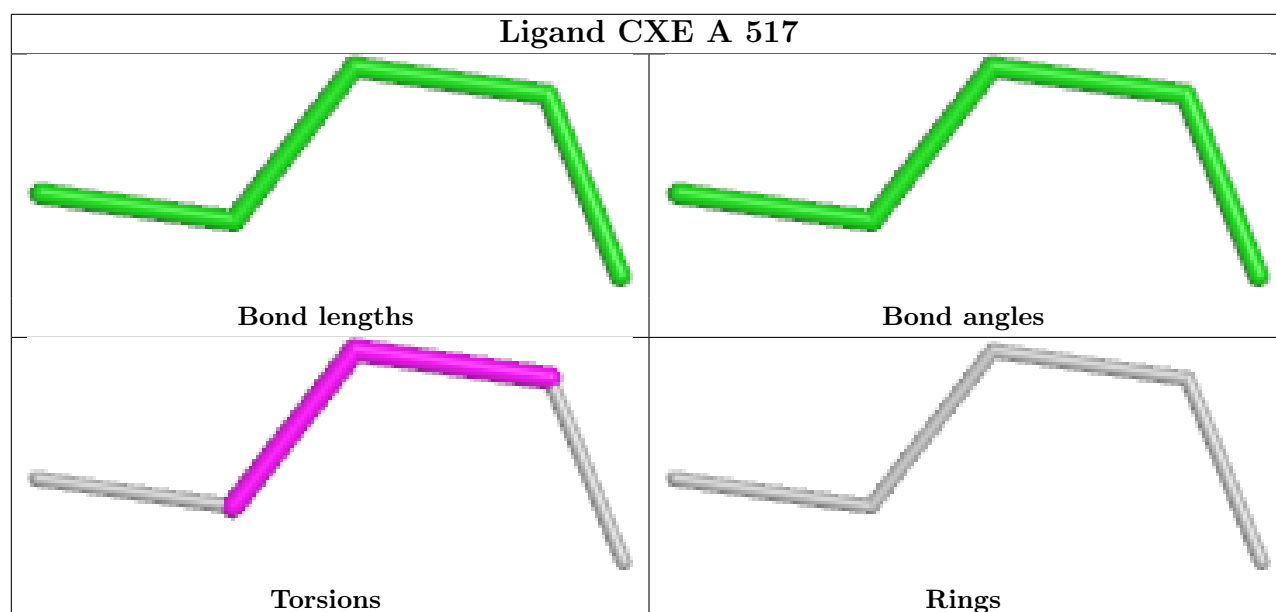
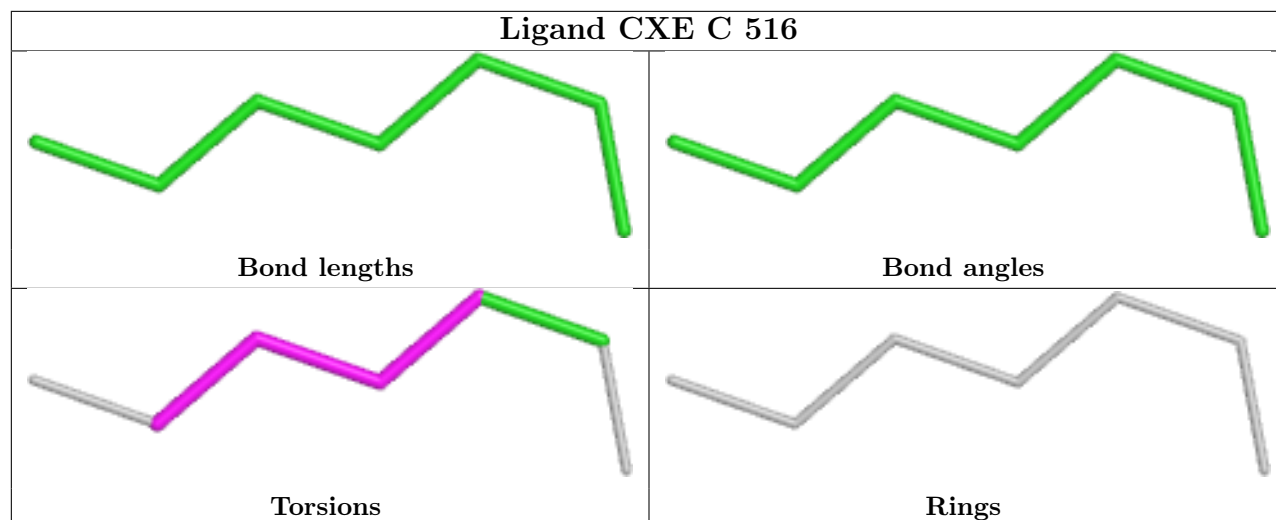


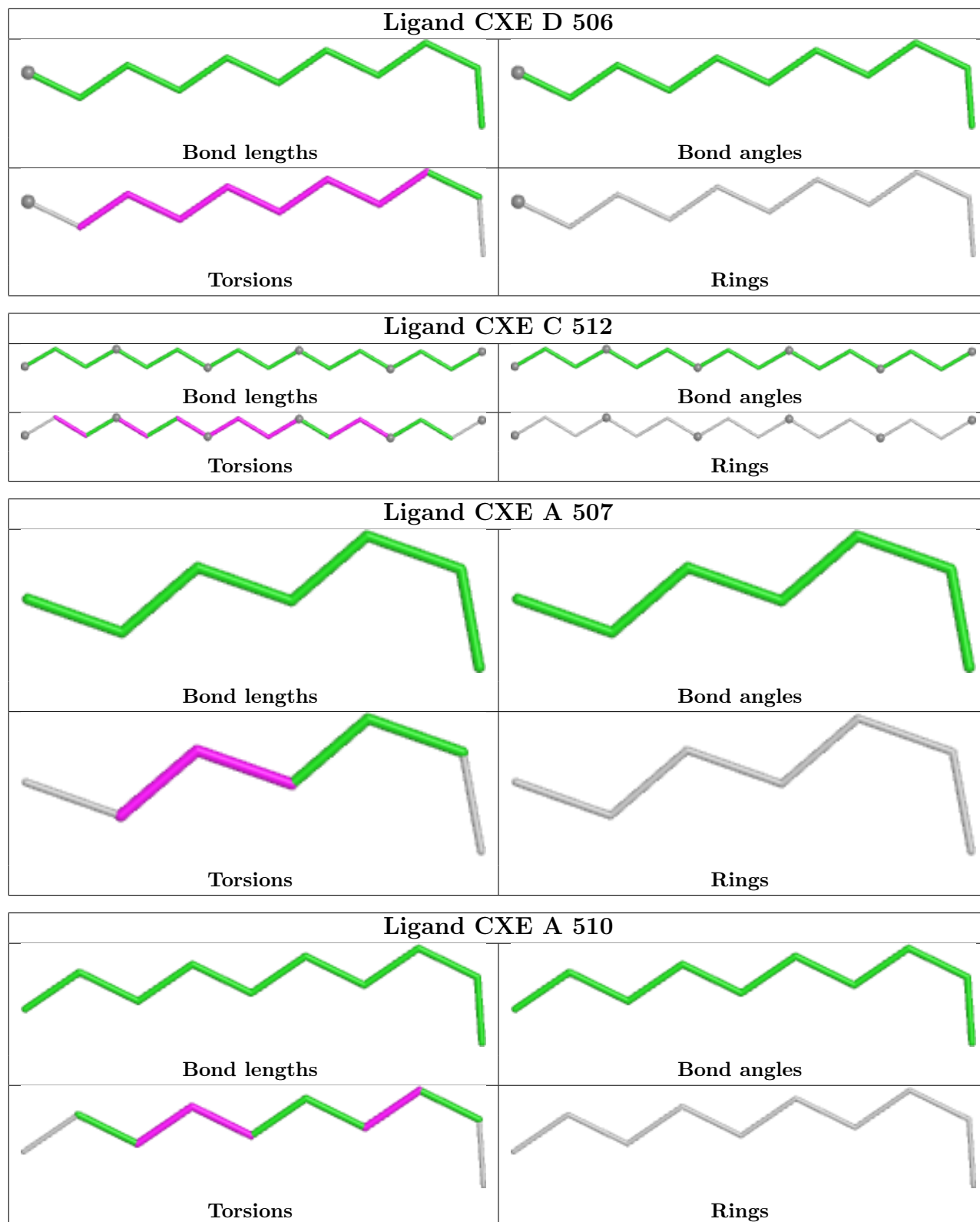


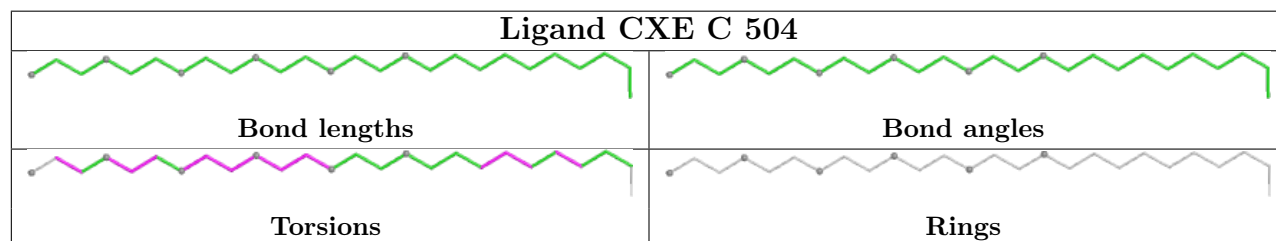
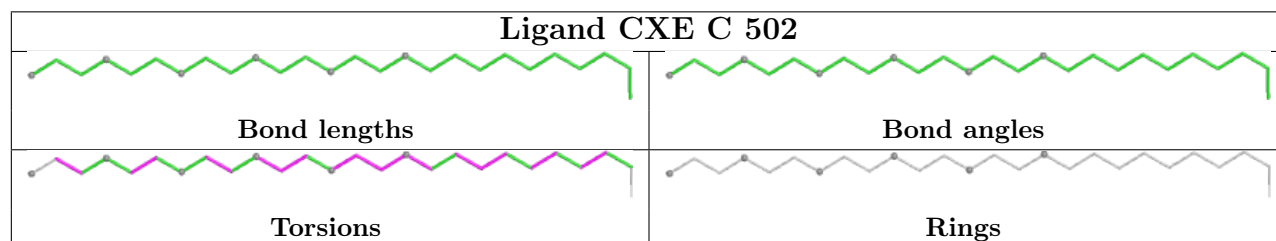
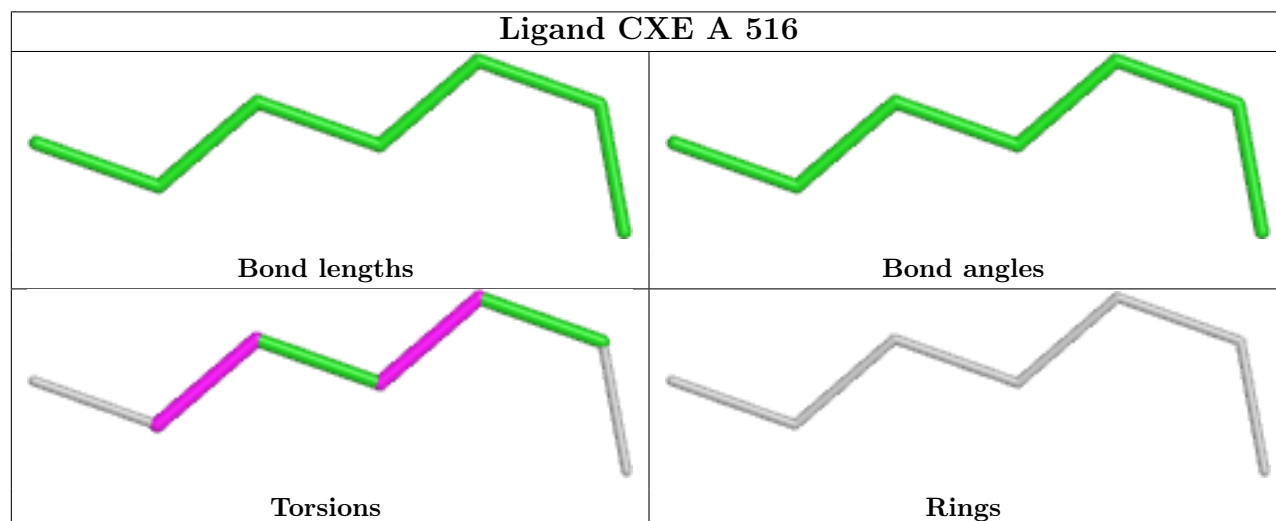
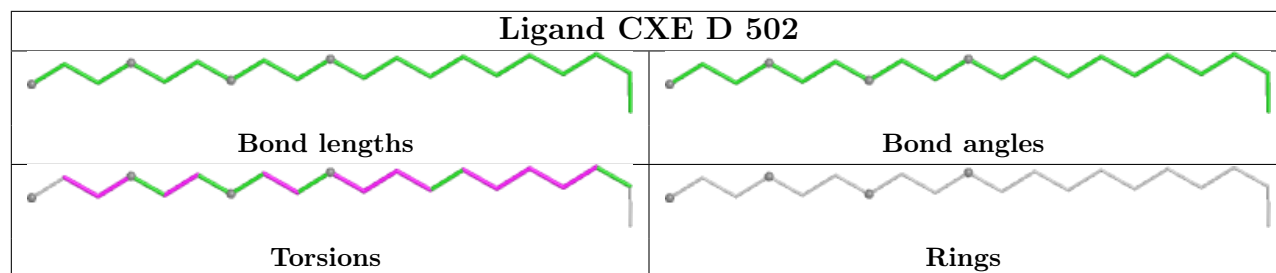


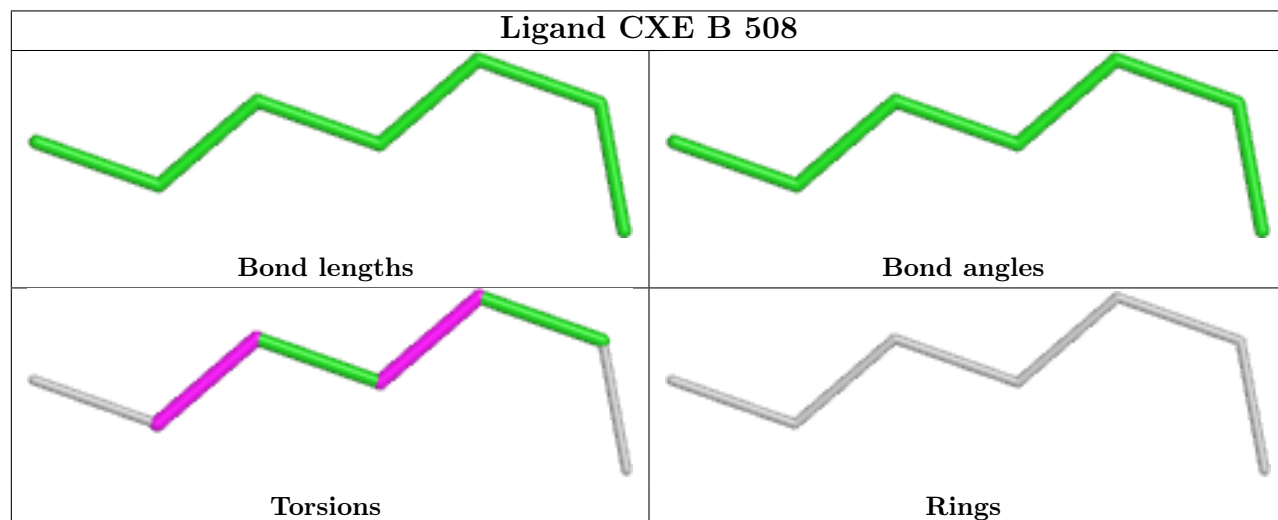
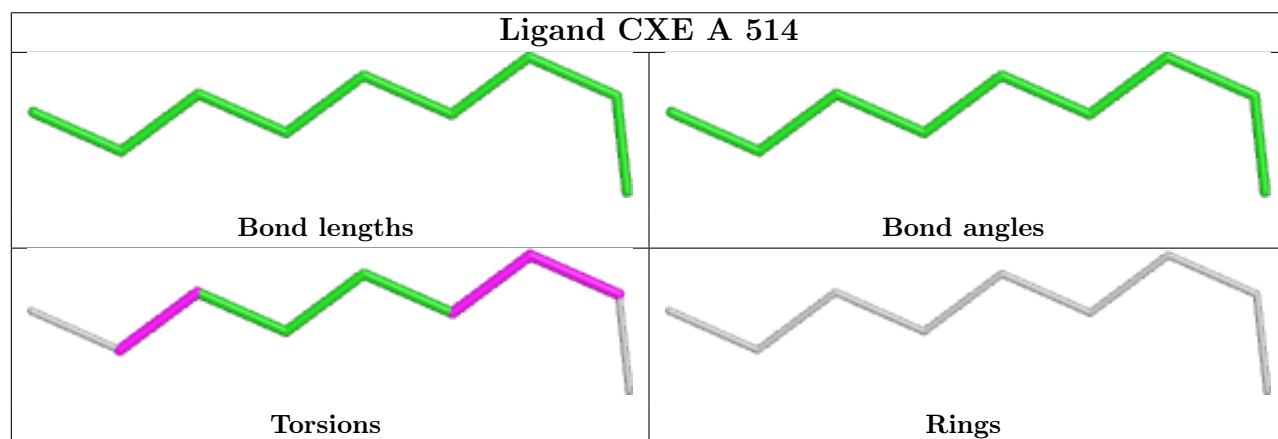
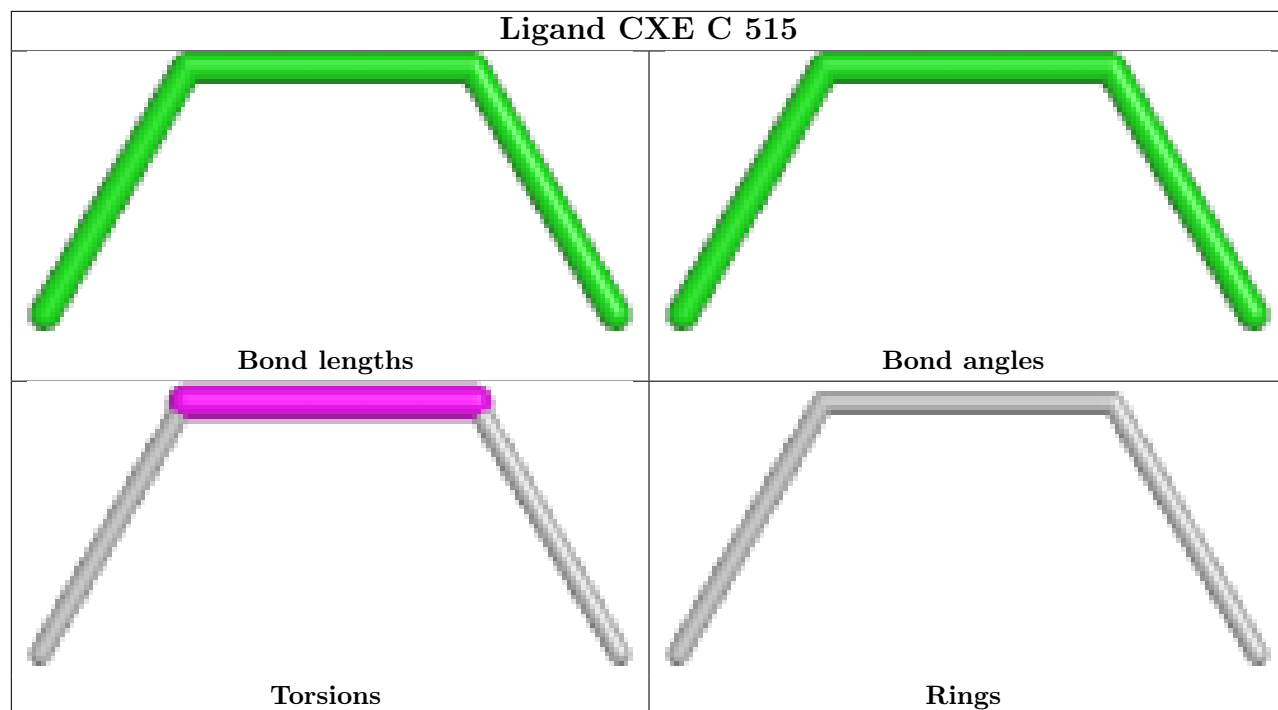


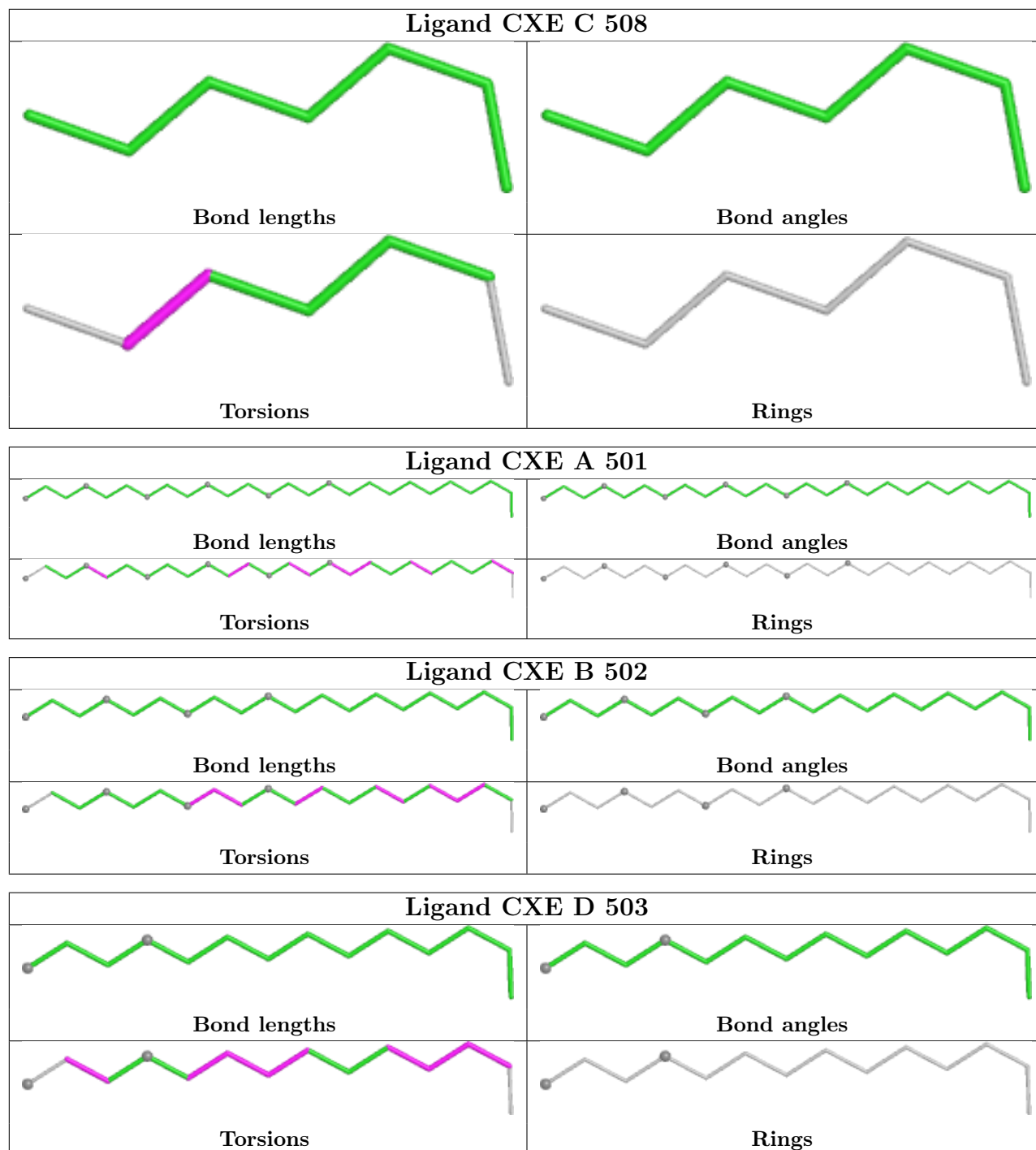


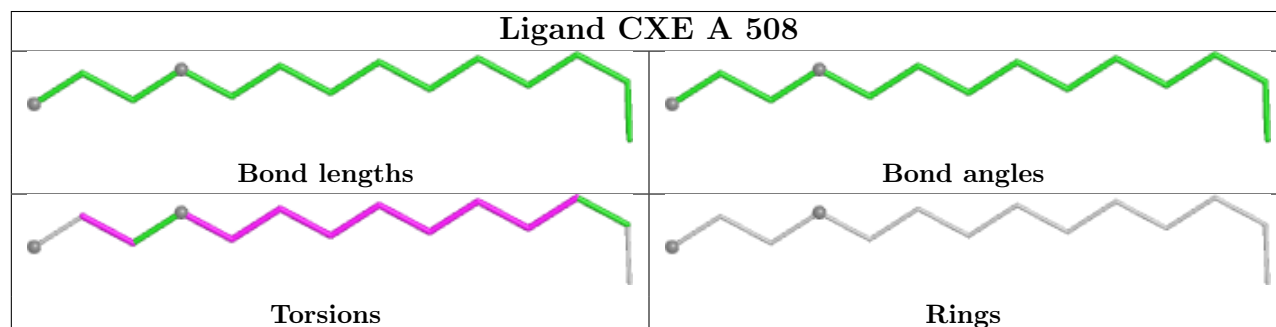
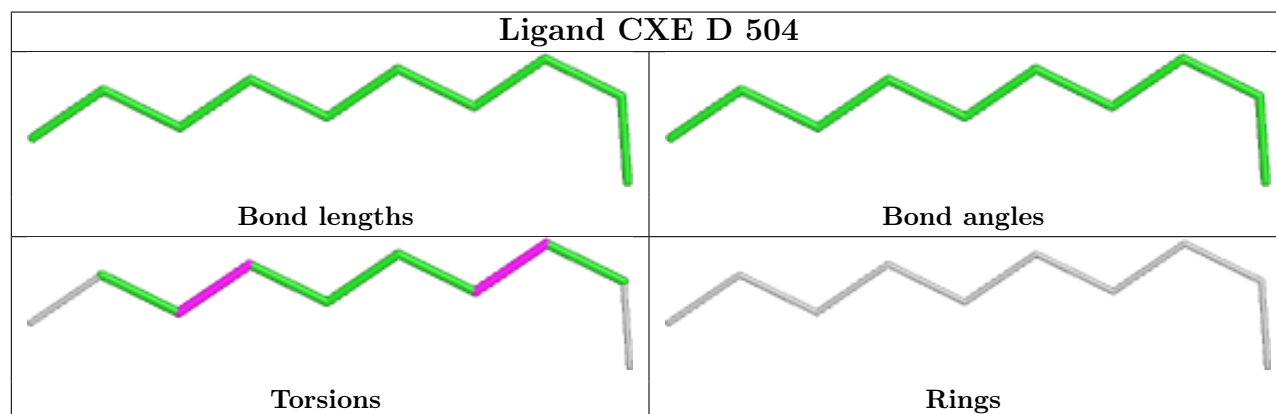
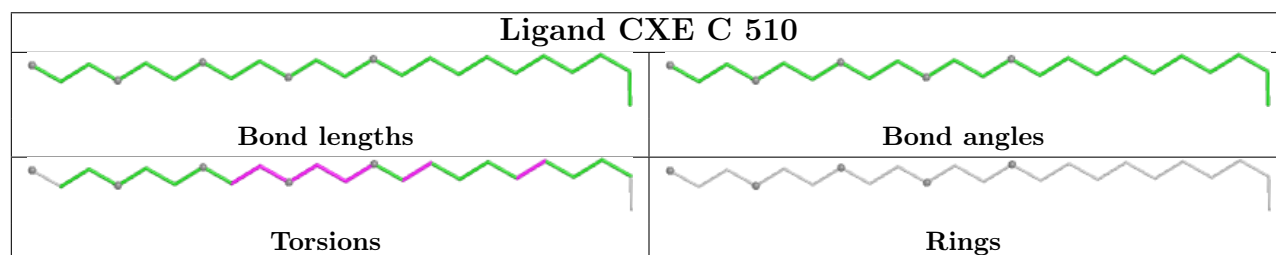
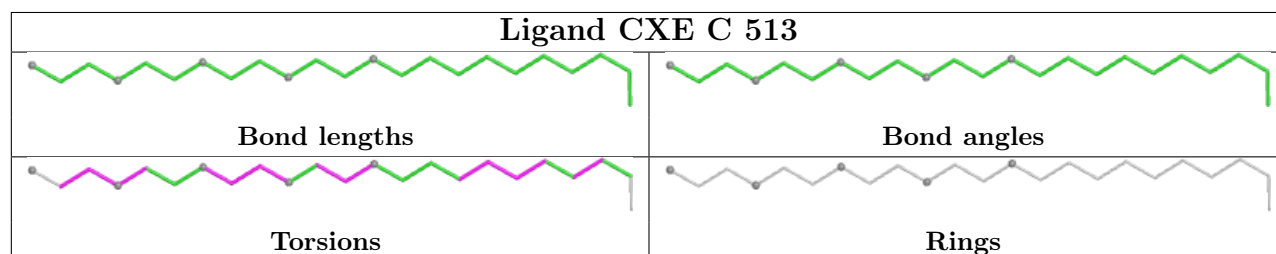
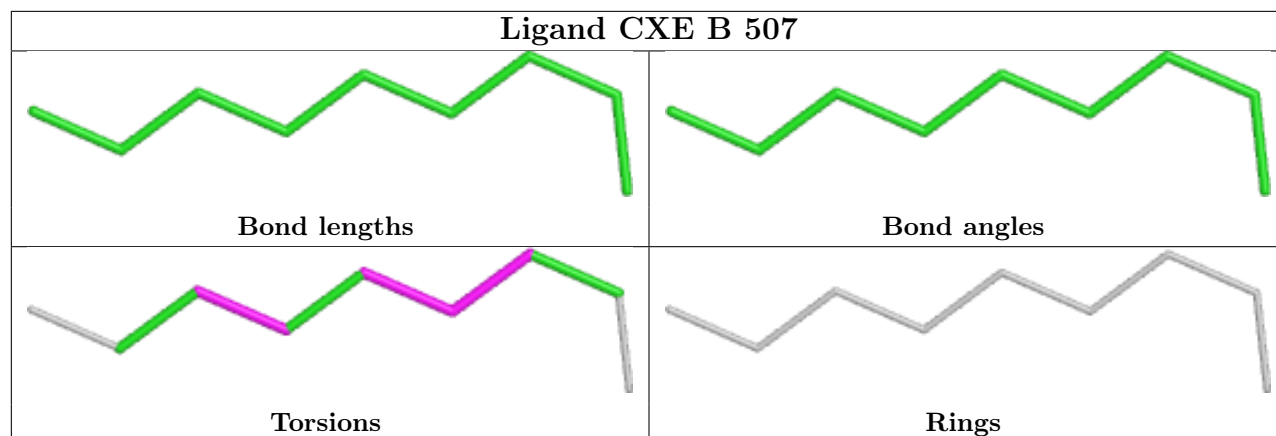


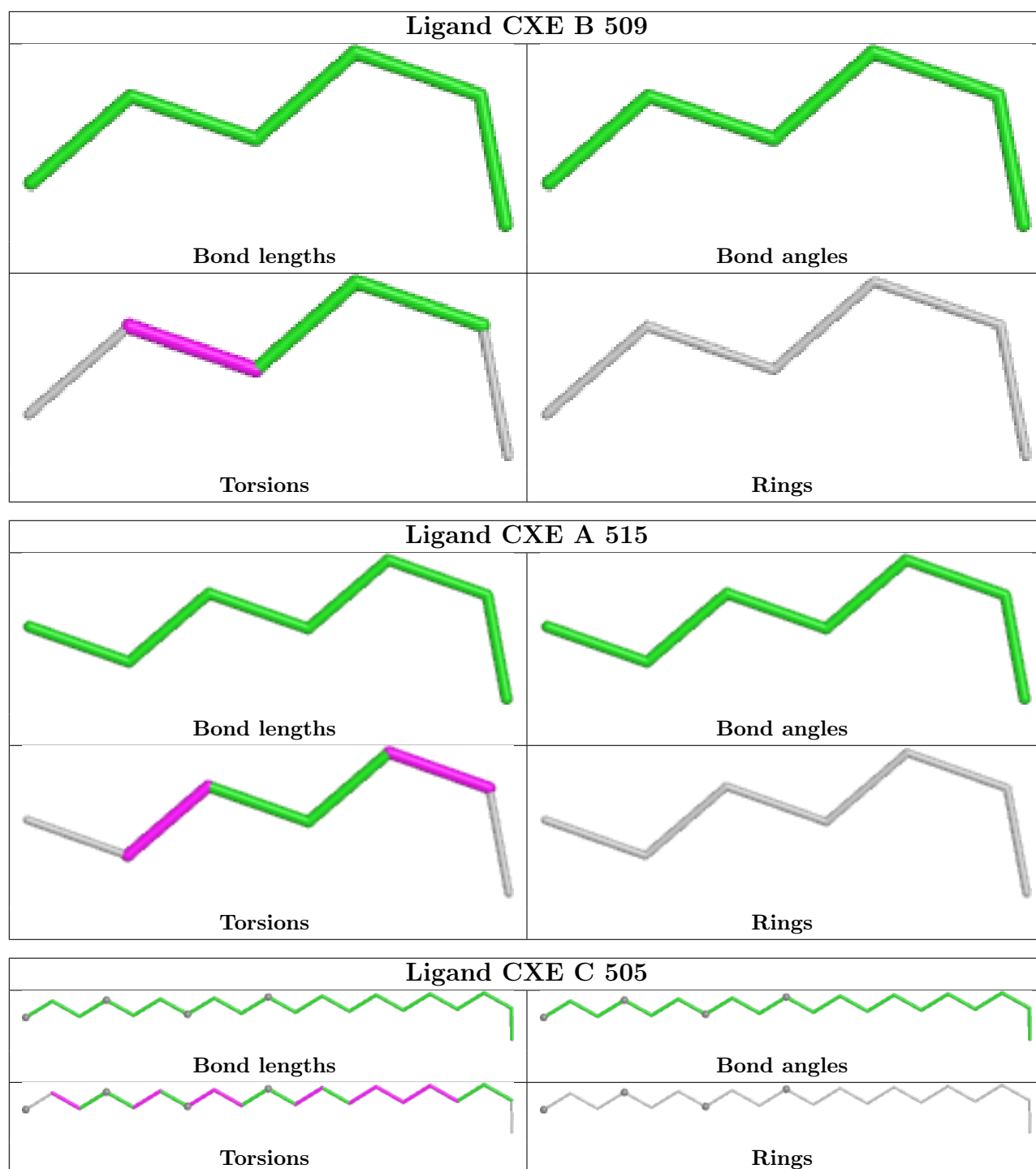












## 5.7 Other polymers [\(i\)](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	453/492 (92%)	0.39	40 (8%) 15 19	19, 37, 89, 146	1 (0%)
1	B	454/492 (92%)	0.44	33 (7%) 21 25	21, 42, 76, 113	0
1	C	452/492 (91%)	0.55	75 (16%) 4 5	19, 35, 105, 142	2 (0%)
1	D	452/492 (91%)	0.94	54 (11%) 9 10	32, 53, 97, 129	2 (0%)
All	All	1811/1968 (92%)	0.58	202 (11%) 10 11	19, 44, 91, 146	5 (0%)

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	357	VAL	5.7
1	B	357	VAL	5.4
1	C	341	PHE	5.4
1	C	421	GLY	5.1
1	C	266	VAL	5.0
1	C	454	THR	5.0
1	C	287	MET	4.8
1	A	357	VAL	4.7
1	C	263	LEU	4.7
1	B	287	MET	4.7
1	D	59	PHE	4.6
1	C	283	TRP	4.5
1	C	426	TRP	4.4
1	D	355	ALA	4.4
1	A	355	ALA	4.4
1	C	370	PRO	4.4
1	D	352	SER	4.3
1	B	229	LEU	4.2
1	C	351	TYR	4.1
1	C	276	VAL	4.1
1	B	355	ALA	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	267	ALA	4.0
1	B	286	THR	4.0
1	C	268	ILE	4.0
1	A	454	THR	4.0
1	C	279	PHE	4.0
1	C	354	SER	4.0
1	C	427	ILE	3.9
1	B	280	THR	3.9
1	C	424	GLY	3.8
1	A	351	TYR	3.7
1	C	357	VAL	3.8
1	C	342	ALA	3.7
1	A	346	ALA	3.6
1	B	4	LYS	3.6
1	D	350	THR	3.6
1	C	261	PHE	3.5
1	B	456	ALA	3.5
1	C	362	LEU	3.5
1	B	358	ILE	3.5
1	D	228	THR	3.4
1	A	456	ALA	3.4
1	C	358	ILE	3.4
1	D	137	ILE	3.4
1	D	229	LEU	3.4
1	A	287	MET	3.3
1	D	358	ILE	3.3
1	A	341	PHE	3.3
1	C	419	THR	3.3
1	B	342	ALA	3.3
1	A	4	LYS	3.3
1	D	127	GLY	3.3
1	C	274	ASN	3.3
1	B	351	TYR	3.3
1	C	59	PHE	3.3
1	D	351	TYR	3.3
1	B	288	LEU	3.3
1	A	340	LEU	3.2
1	D	122	LEU	3.2
1	D	287	MET	3.2
1	A	232	PHE	3.1
1	A	231	ASP	3.1
1	A	366	LEU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	422	LEU	3.1
1	D	63	PHE	3.1
1	C	349	PHE	3.1
1	C	260	MET	3.1
1	C	271	GLY	3.1
1	D	49	GLY	3.1
1	C	270	ALA	3.1
1	C	278	VAL	3.1
1	D	135	LEU	3.1
1	A	271	GLY	3.0
1	B	59	PHE	3.0
1	C	269	THR	3.0
1	A	230	ARG	3.0
1	C	365	ALA	3.0
1	A	288	LEU	3.0
1	C	368	THR	3.0
1	A	349	PHE	2.9
1	C	128	ALA	2.9
1	C	420	LEU	2.9
1	C	425	VAL	2.9
1	D	133	VAL	2.9
1	C	350	THR	2.9
1	D	128	ALA	2.9
1	D	164	GLY	2.9
1	C	277	ALA	2.9
1	D	283	TRP	2.9
1	C	414	PHE	2.8
1	B	3	GLU	2.8
1	B	5	THR	2.8
1	A	283	TRP	2.8
1	C	353	GLU	2.8
1	B	127	GLY	2.8
1	B	232	PHE	2.8
1	C	415	VAL	2.8
1	C	264	ASN	2.7
1	D	354	SER	2.7
1	A	348	LEU	2.7
1	D	353	GLU	2.7
1	B	273	GLU	2.7
1	B	126	MET	2.7
1	C	411	ALA	2.7
1	A	335	VAL	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	234	PRO	2.7
1	A	126	MET	2.7
1	D	87	ALA	2.6
1	D	454	THR	2.6
1	D	126	MET	2.6
1	C	122	LEU	2.6
1	D	132	ALA	2.6
1	D	214	ALA	2.6
1	B	284	ARG	2.6
1	A	339	MET	2.6
1	C	363	ILE	2.6
1	C	355	ALA	2.6
1	C	126	MET	2.6
1	D	5	THR	2.6
1	D	264	ASN	2.5
1	B	283	TRP	2.5
1	C	343	PRO	2.5
1	C	418	THR	2.5
1	B	290	ILE	2.5
1	C	369	LEU	2.5
1	D	288	LEU	2.5
1	D	232	PHE	2.5
1	C	340	LEU	2.5
1	D	129	LYS	2.5
1	A	365	ALA	2.5
1	B	354	SER	2.4
1	B	362	LEU	2.4
1	A	274	ASN	2.4
1	C	4	LYS	2.4
1	C	143	LEU	2.4
1	D	224	TYR	2.4
1	B	228	THR	2.4
1	A	338	ILE	2.4
1	D	190	THR	2.4
1	A	276	VAL	2.4
1	A	380	MET	2.4
1	D	119	ILE	2.4
1	D	123	PHE	2.4
1	D	218	PHE	2.4
1	D	101	LEU	2.4
1	C	367	ARG	2.4
1	C	272	GLY	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	354	SER	2.3
1	D	311	ARG	2.3
1	B	353	GLU	2.3
1	C	345	VAL	2.3
1	D	349	PHE	2.3
1	C	288	LEU	2.3
1	D	143	LEU	2.3
1	D	215	TYR	2.3
1	C	284	ARG	2.3
1	A	261	PHE	2.3
1	B	372	PHE	2.3
1	A	117	PRO	2.3
1	A	358	ILE	2.3
1	C	372	PHE	2.2
1	D	440	GLY	2.2
1	D	145	ALA	2.2
1	A	359	LYS	2.2
1	B	129	LYS	2.2
1	C	127	GLY	2.2
1	C	360	GLY	2.2
1	D	356	GLN	2.2
1	A	363	ILE	2.2
1	D	11	LEU	2.2
1	A	361	ASP	2.2
1	B	356	GLN	2.2
1	A	419	THR	2.2
1	A	455	SER	2.2
1	D	216	TRP	2.2
1	B	289	GLY	2.2
1	B	46	SER	2.2
1	A	362	LEU	2.1
1	B	311	ARG	2.1
1	C	423	ARG	2.1
1	D	124	ARG	2.1
1	A	347	TYR	2.1
1	A	293	ILE	2.1
1	C	413	ILE	2.1
1	D	53	LEU	2.1
1	C	346	ALA	2.1
1	C	364	SER	2.1
1	C	347	TYR	2.1
1	C	352	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	420	LEU	2.1
1	C	262	PHE	2.1
1	C	275	GLY	2.1
1	D	192	GLY	2.1
1	C	125	SER	2.0
1	C	259	ALA	2.0
1	D	96	VAL	2.0
1	D	148	PHE	2.0
1	B	233	SER	2.0
1	C	286	THR	2.0
1	D	282	ALA	2.0
1	C	344	GLN	2.0
1	C	453	LYS	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CXE	B	511	6/26	0.60	0.46	34,38,39,42	6
2	CXE	B	509	6/26	0.66	0.48	32,36,42,45	6
2	CXE	C	514	17/26	0.69	0.22	50,70,93,93	0
2	CXE	C	505	20/26	0.71	0.20	46,62,82,83	0
2	CXE	A	513	20/26	0.71	0.22	42,74,102,106	0
2	CXE	A	511	10/26	0.72	0.20	58,66,74,74	0
2	CXE	C	504	26/26	0.72	0.17	50,72,102,105	0
2	CXE	A	508	14/26	0.74	0.17	63,78,100,100	0
2	CXE	C	503	26/26	0.75	0.18	47,57,74,78	0
2	CXE	A	517	5/26	0.75	0.23	56,60,63,68	0

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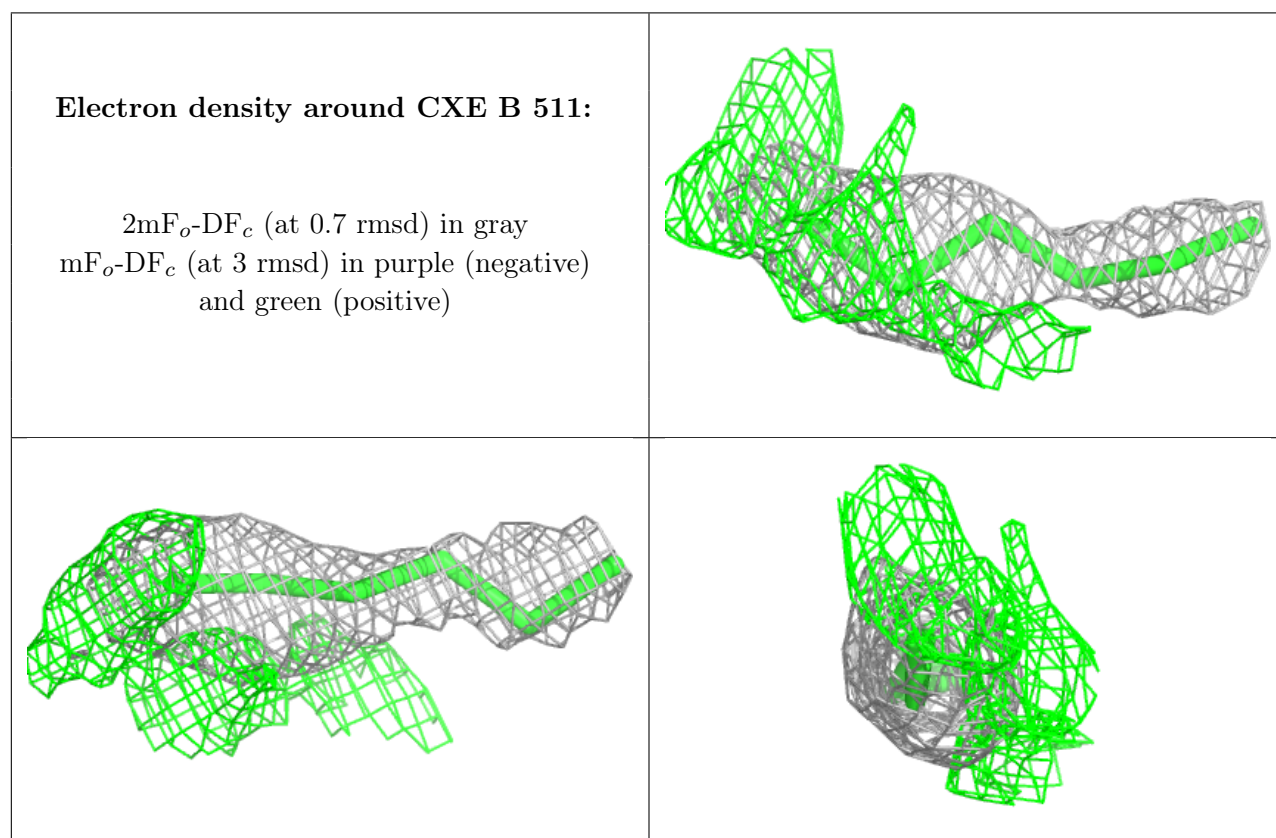
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CXE	A	503	26/26	0.75	0.20	65,77,83,85	0
2	CXE	C	507	10/26	0.75	0.19	60,68,79,80	0
2	CXE	C	513	23/26	0.75	0.17	57,67,81,85	0
2	CXE	A	509	23/26	0.75	0.22	56,83,102,104	0
2	CXE	A	516	7/26	0.76	0.19	52,57,70,73	0
2	CXE	C	509	17/26	0.77	0.19	54,76,85,95	0
2	CXE	D	504	10/26	0.77	0.23	55,59,73,74	0
2	CXE	C	502	26/26	0.79	0.14	40,76,83,87	0
2	CXE	A	514	9/26	0.79	0.17	55,62,69,73	0
2	CXE	C	516	7/26	0.79	0.20	51,65,67,68	0
2	CXE	C	512	16/26	0.79	0.19	38,57,82,89	0
2	CXE	C	506	15/26	0.81	0.17	37,47,71,75	0
2	CXE	B	502	20/26	0.81	0.18	36,50,62,65	0
2	CXE	B	504	11/26	0.81	0.18	36,74,78,81	0
2	CXE	C	510	23/26	0.81	0.19	49,73,80,88	0
2	CXE	C	511	10/26	0.81	0.21	48,56,65,67	0
2	CXE	B	510	6/26	0.82	0.18	62,69,71,72	0
2	CXE	B	505	10/26	0.82	0.17	46,60,72,77	0
2	CXE	C	508	7/26	0.83	0.18	52,59,64,66	0
2	CXE	B	506	17/26	0.83	0.16	56,70,84,84	0
2	CXE	A	505	10/26	0.83	0.25	38,42,47,63	10
2	CXE	D	506	11/26	0.83	0.19	64,68,87,91	0
2	CXE	D	507	11/26	0.83	0.17	48,58,67,70	0
2	CXE	A	510	10/26	0.84	0.16	36,63,68,69	0
2	CXE	B	503	17/26	0.84	0.17	46,53,66,68	3
2	CXE	B	512	9/26	0.84	0.15	44,53,62,65	0
2	CXE	A	515	7/26	0.84	0.16	38,53,65,65	0
2	CXE	A	504	20/26	0.85	0.15	43,61,77,81	0
2	CXE	B	507	9/26	0.85	0.16	36,61,73,84	0
2	CXE	D	501	11/26	0.85	0.16	41,46,65,65	0
2	CXE	D	508	5/26	0.85	0.14	56,57,57,58	0
2	CXE	D	502	20/26	0.86	0.20	38,48,56,58	10
2	CXE	B	508	7/26	0.86	0.14	44,52,67,68	0
2	CXE	D	505	14/26	0.86	0.17	49,66,77,78	0
2	CXE	A	502	26/26	0.86	0.15	29,48,74,81	0
2	CXE	A	501	26/26	0.86	0.13	35,49,60,64	0
2	CXE	A	507	7/26	0.86	0.16	42,52,59,62	0
2	CXE	A	512	6/26	0.88	0.17	34,49,53,65	0
2	CXE	C	501	26/26	0.88	0.15	26,43,88,95	0
2	CXE	B	501	26/26	0.88	0.13	35,50,77,86	0
2	CXE	C	515	4/26	0.88	0.14	48,50,54,66	0
2	CXE	D	503	14/26	0.90	0.13	53,61,65,76	0

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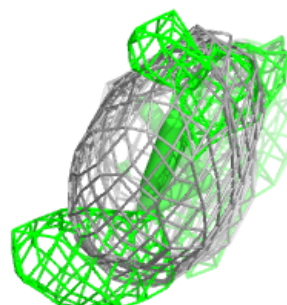
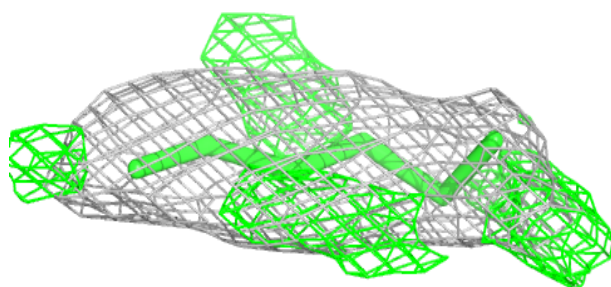
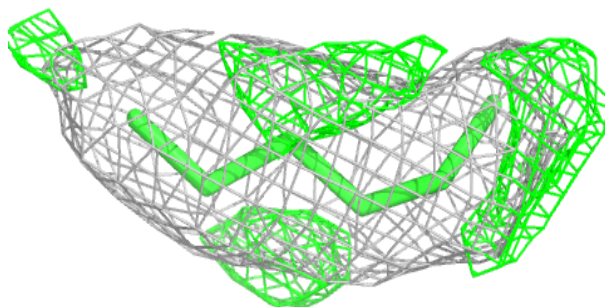
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CXE	A	506	20/26	0.90	0.11	24,39,57,58	0
3	CL	A	518	1/1	0.98	0.05	29,29,29,29	0
3	CL	A	519	1/1	0.99	0.03	37,37,37,37	0

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.

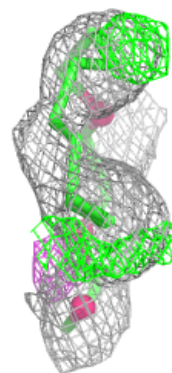
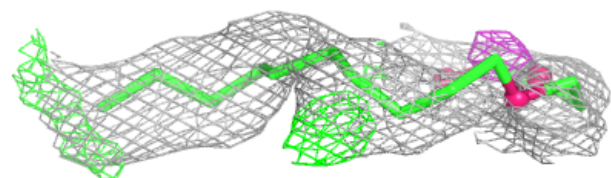
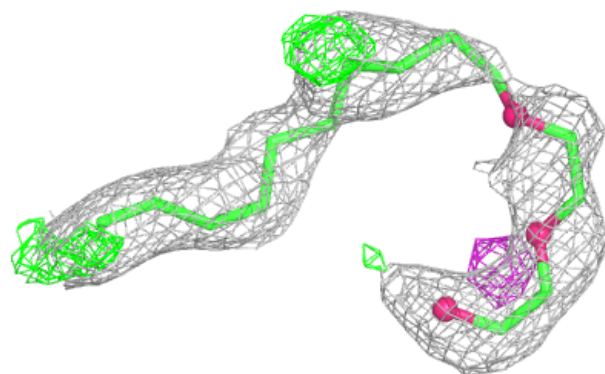


**Electron density around CXE B 509:**

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

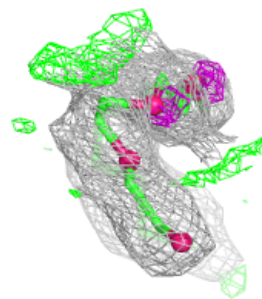
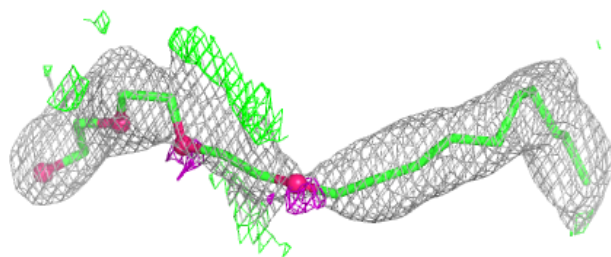
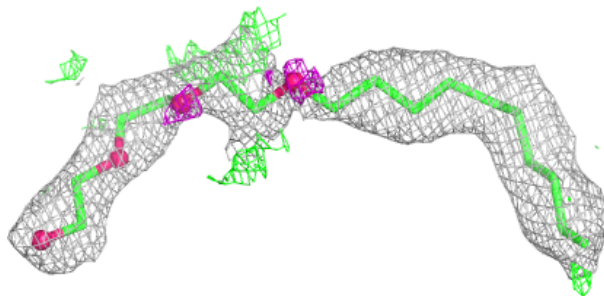
**Electron density around CXE C 514:**

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

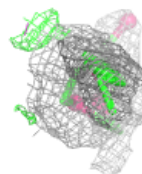
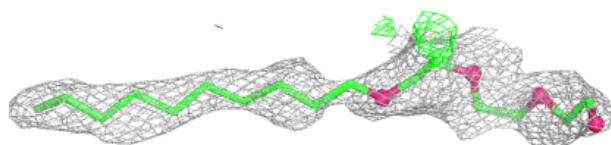
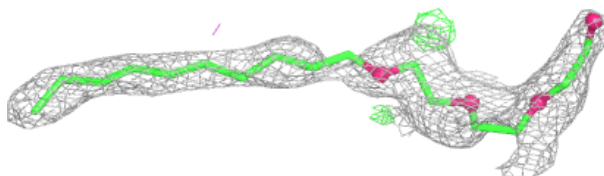


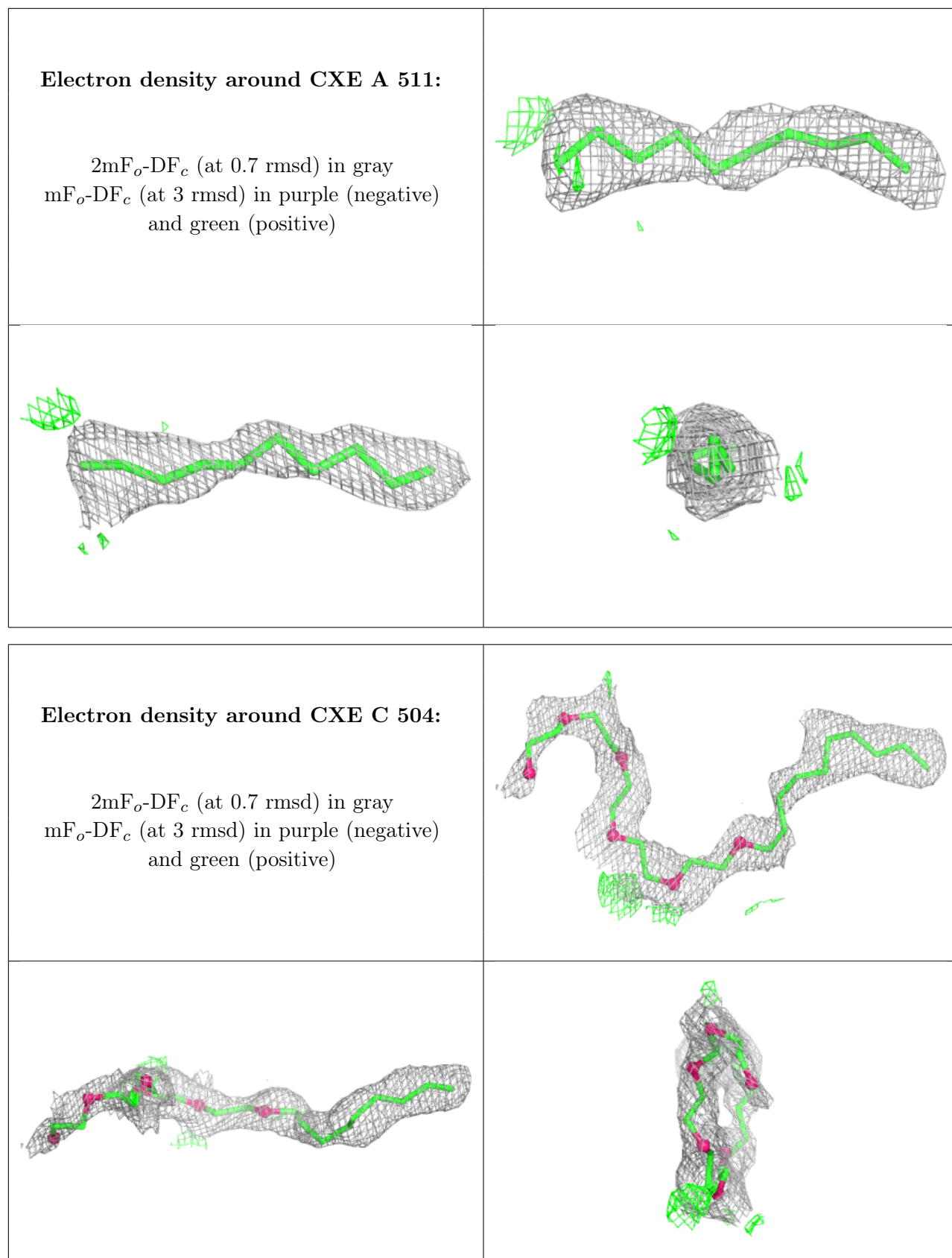
**Electron density around CXE C 505:**

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and green (positive)

**Electron density around CXE A 513:**

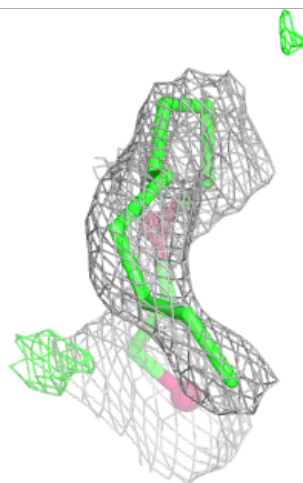
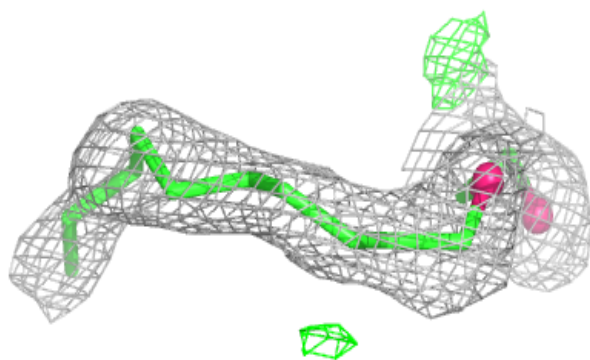
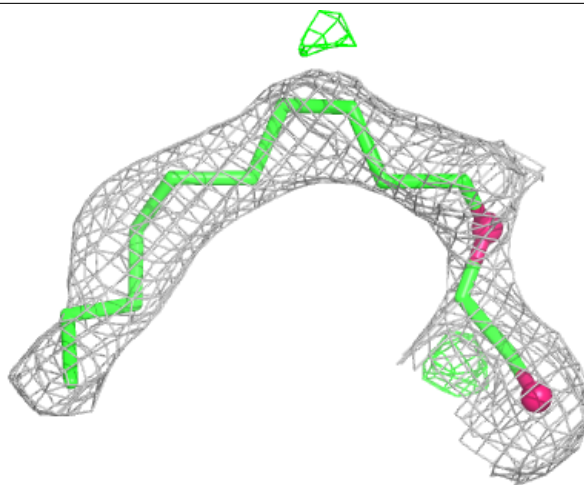
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





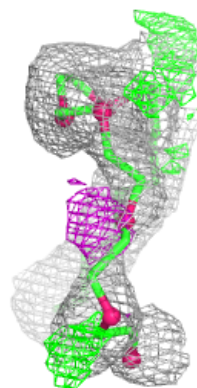
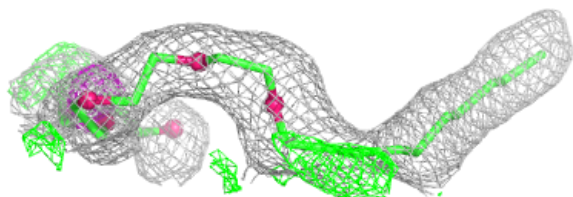
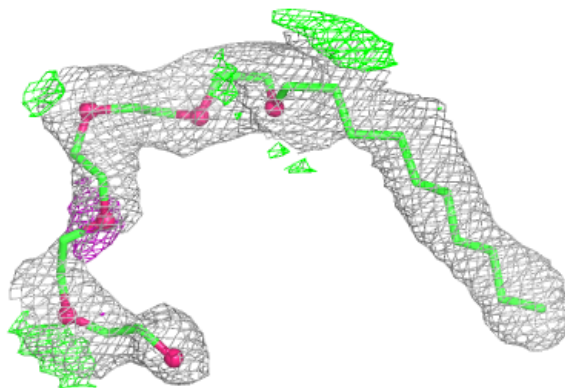
**Electron density around CXE A 508:**

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and green (positive)

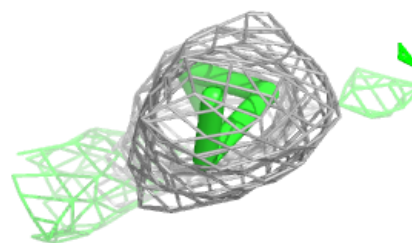
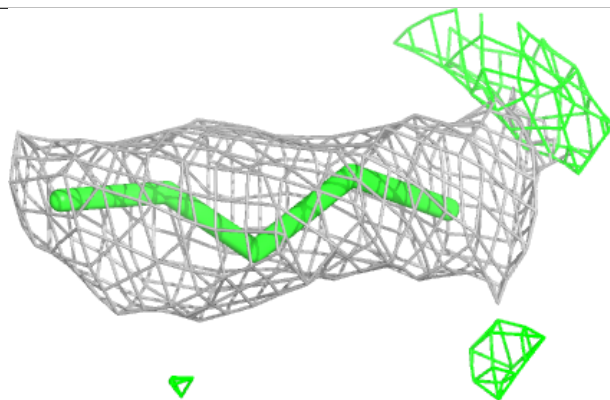
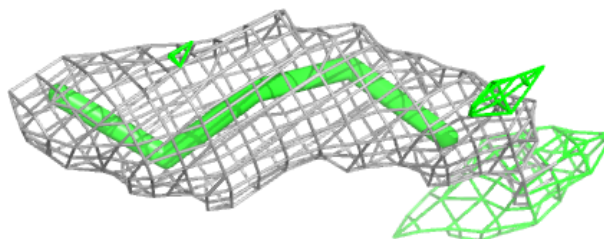


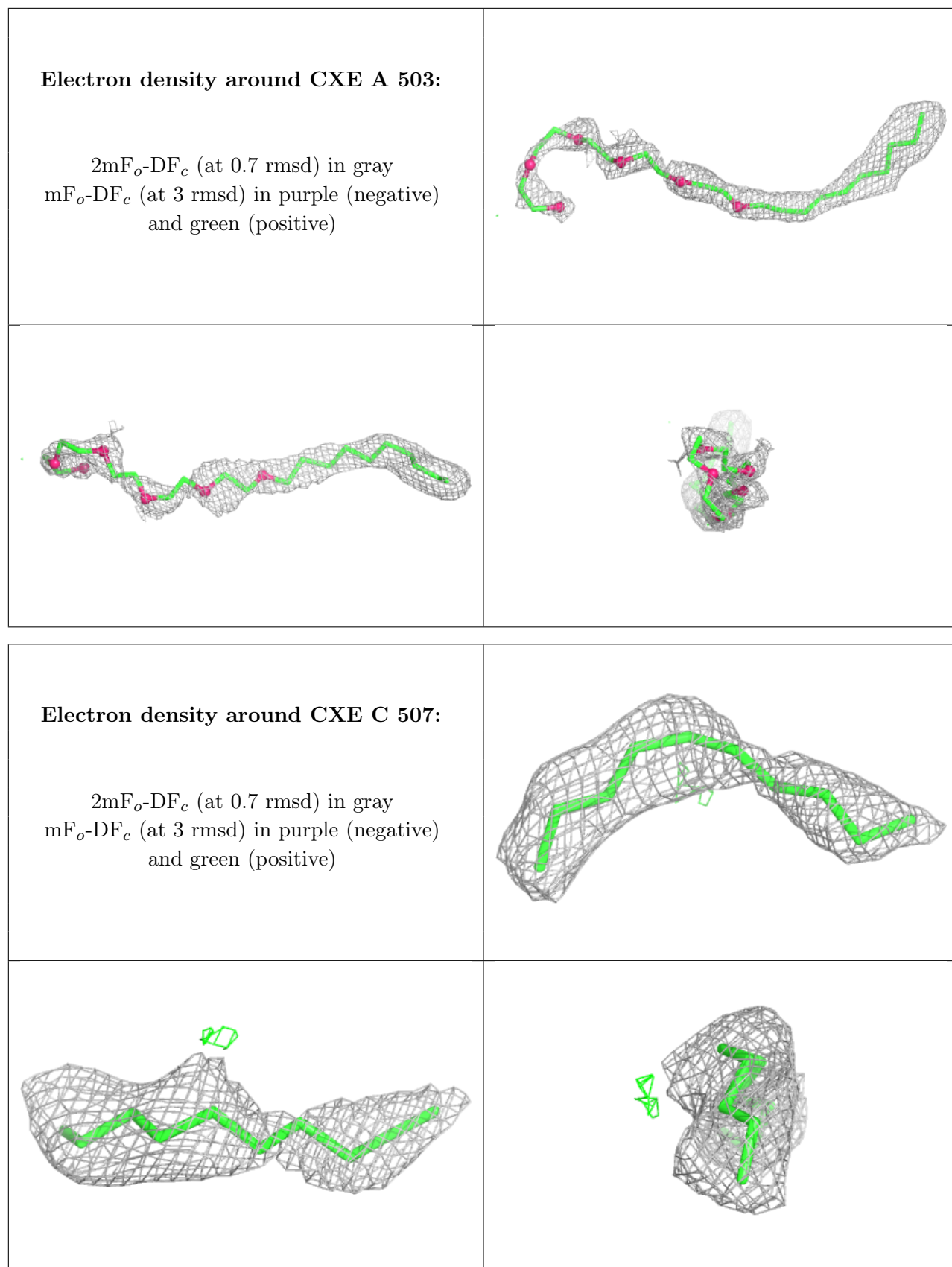
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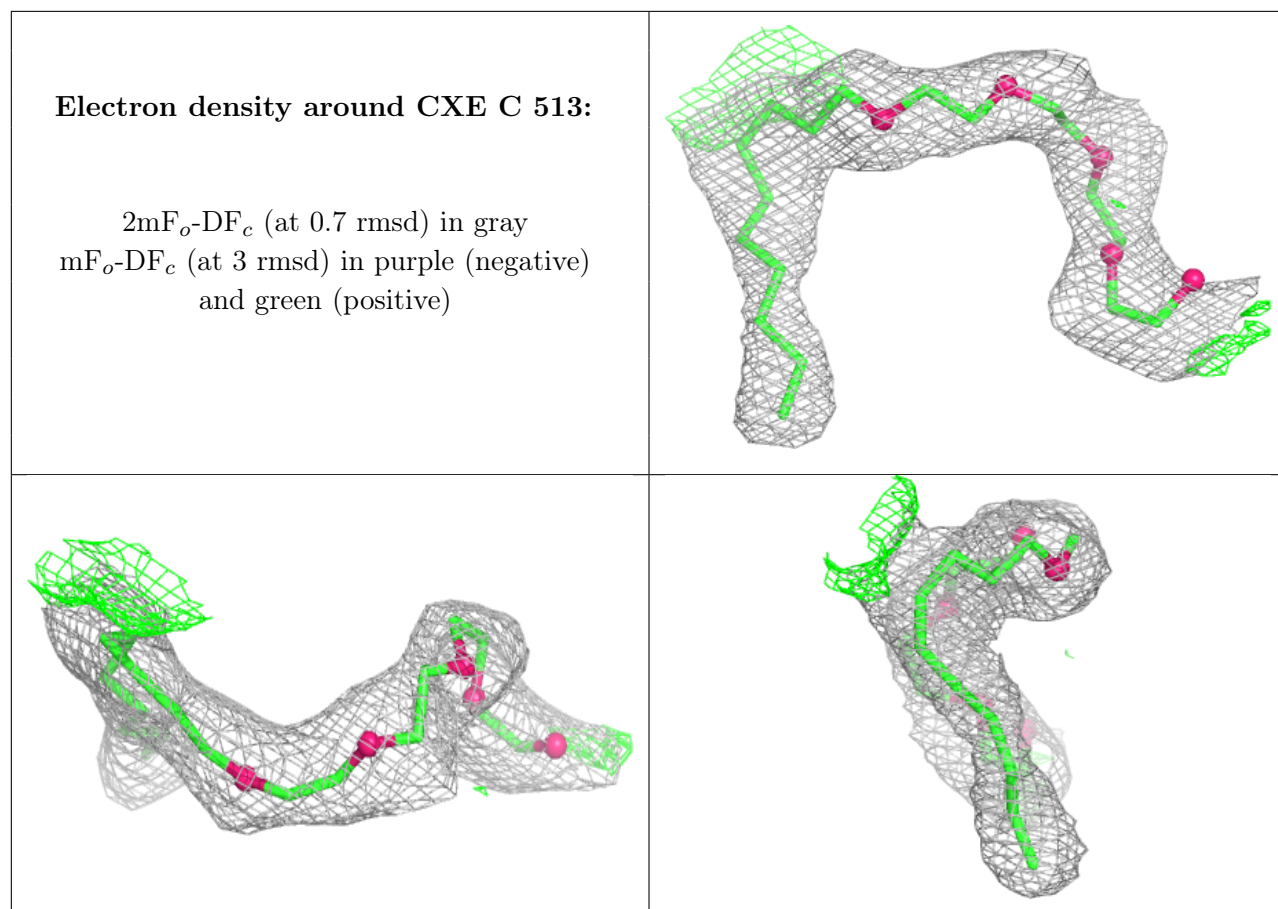
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

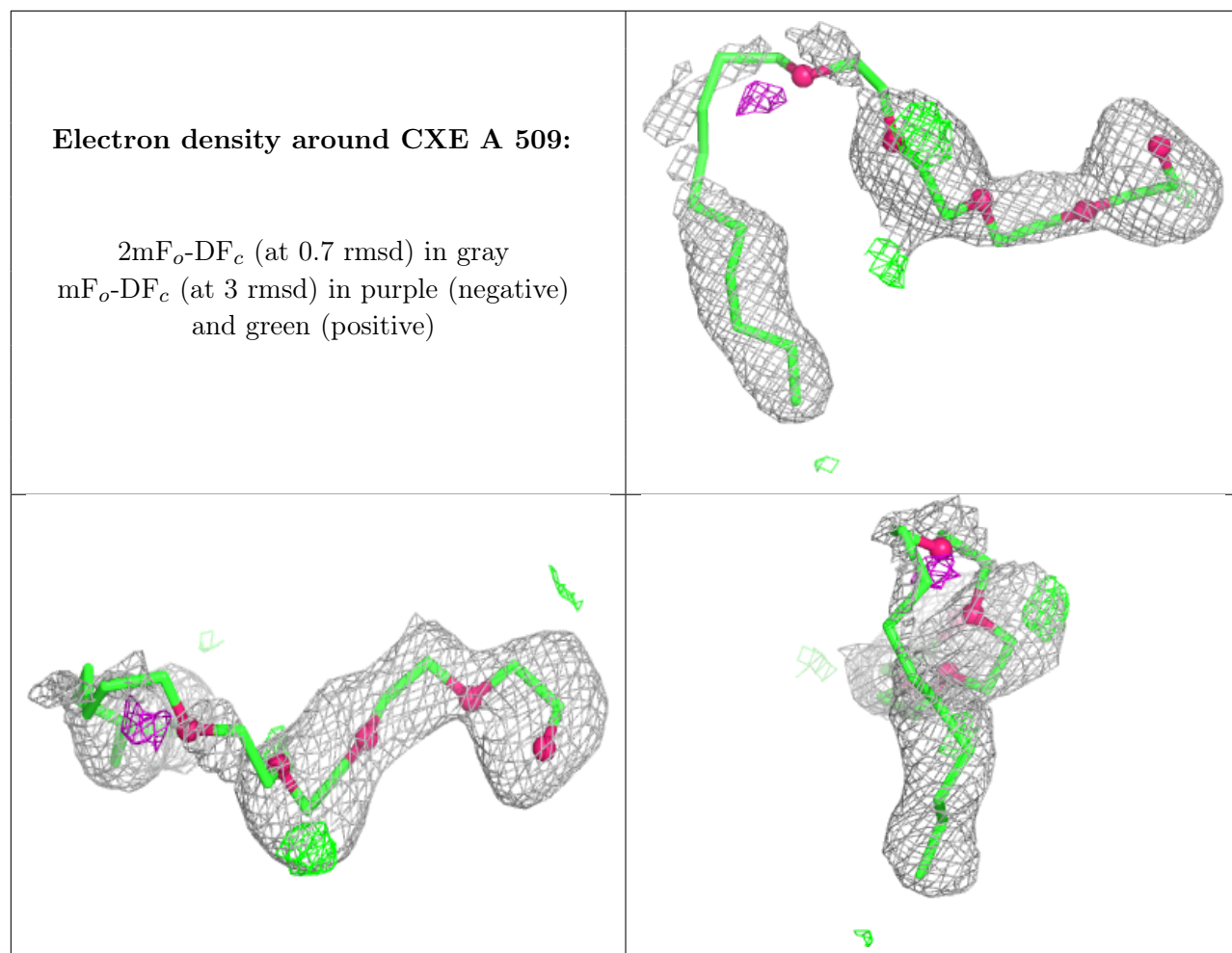
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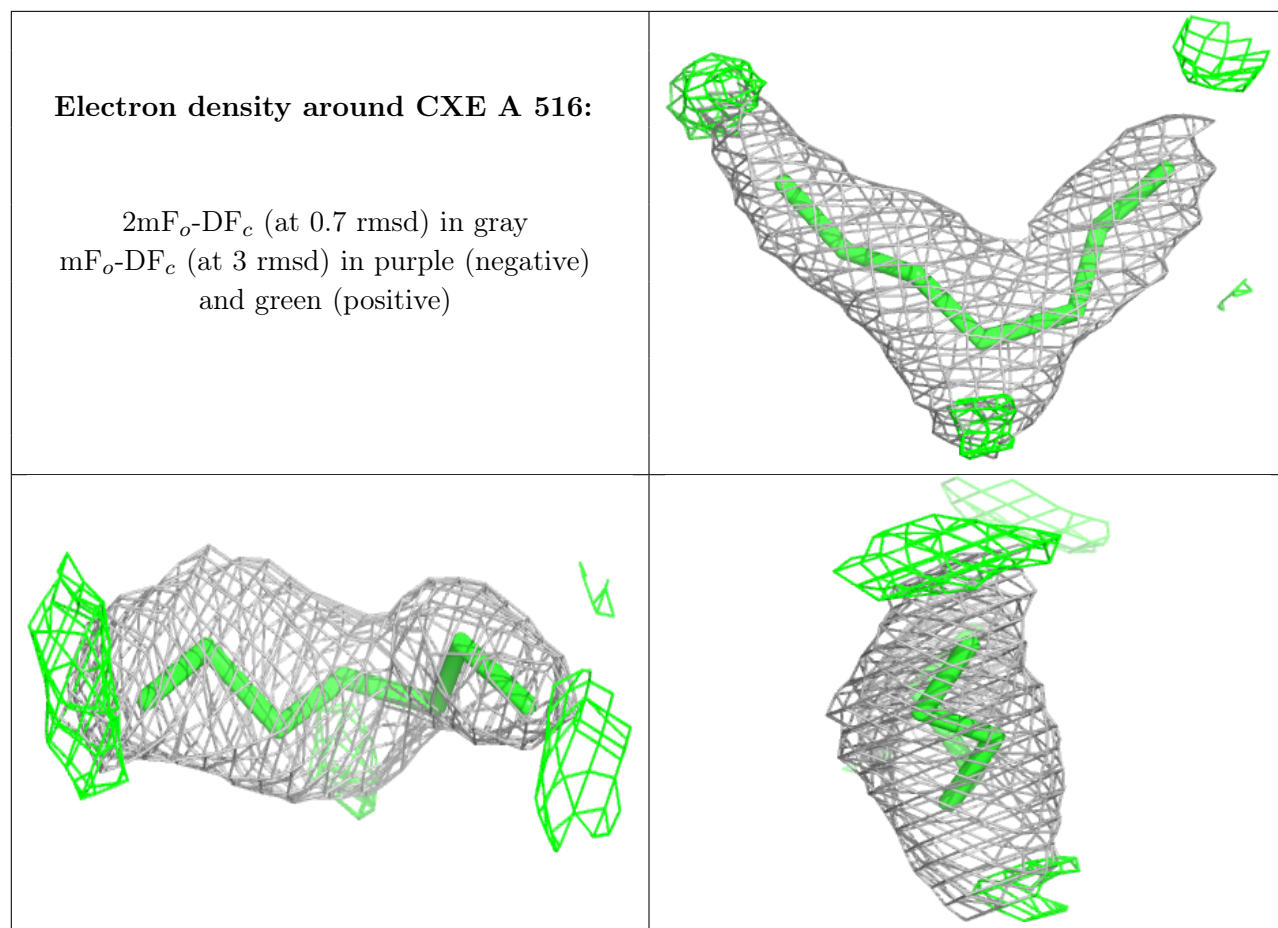
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and green (positive)





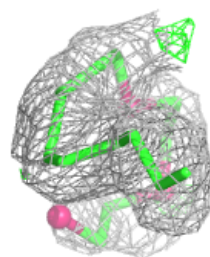
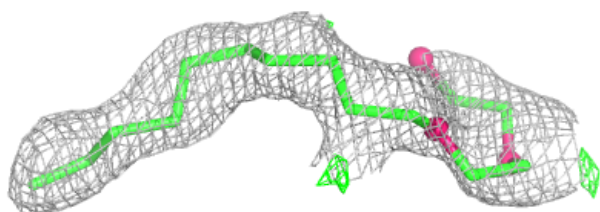
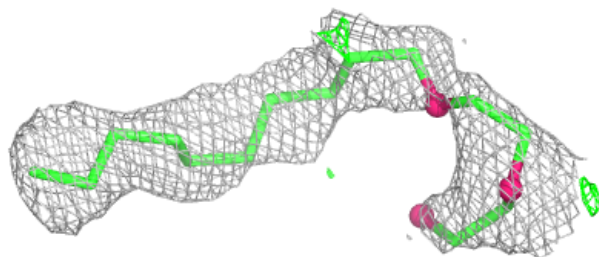




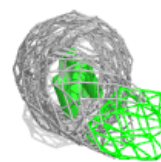
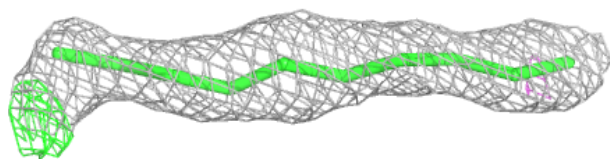
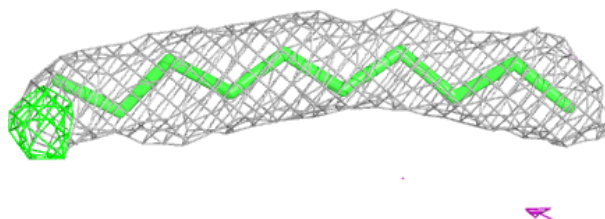


**Electron density around CXE C 509:**

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and green (positive)

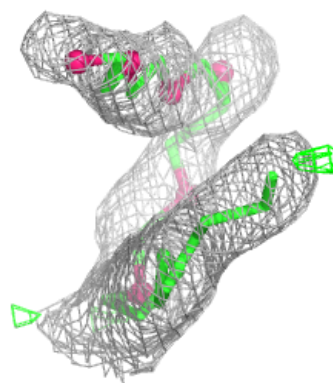
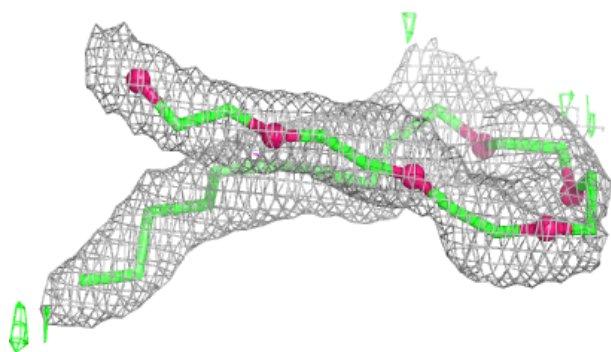
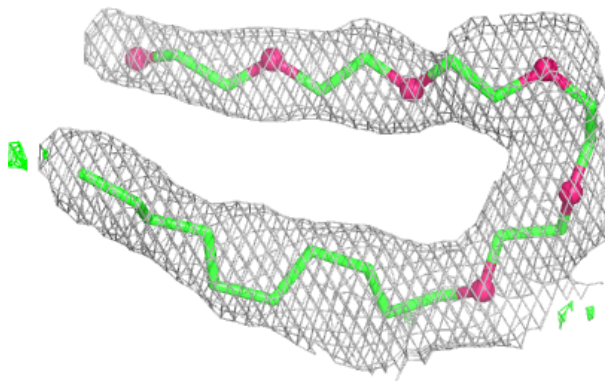
**Electron density around CXE D 504:**

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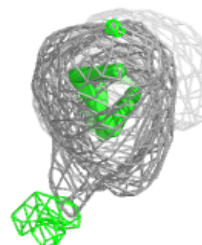
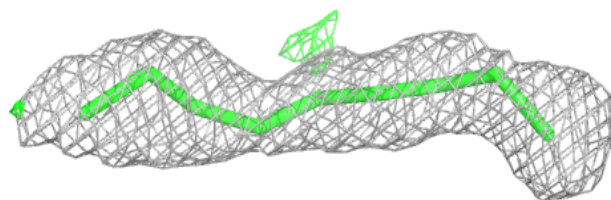
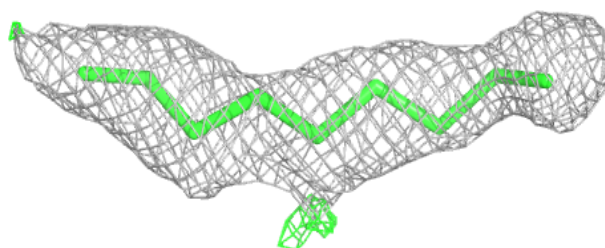


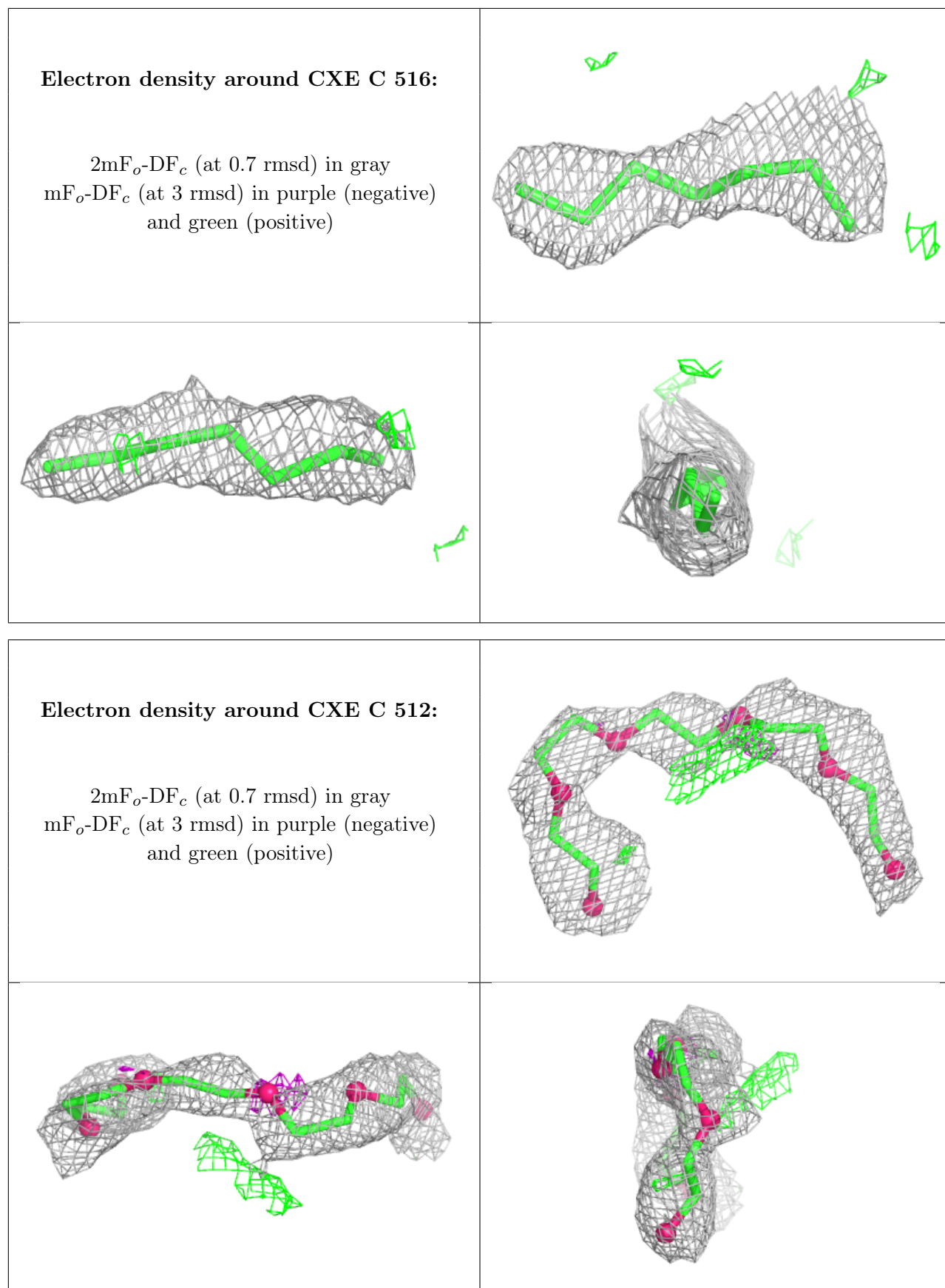
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and green (positive)

**Electron density around CXE A 514:**

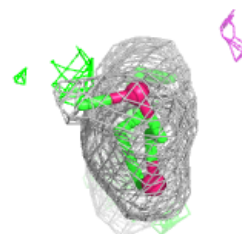
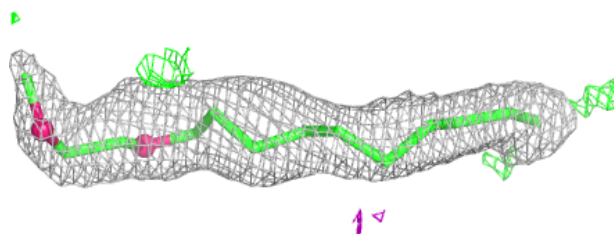
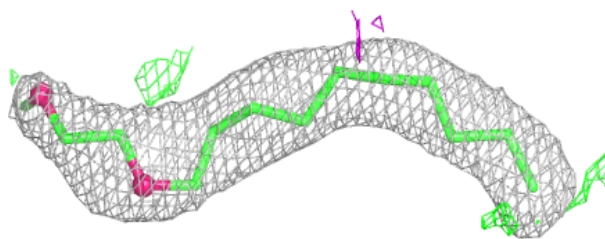
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



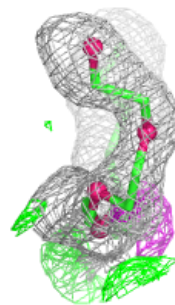
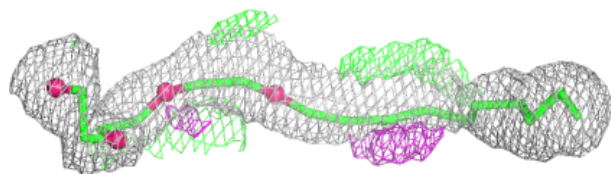
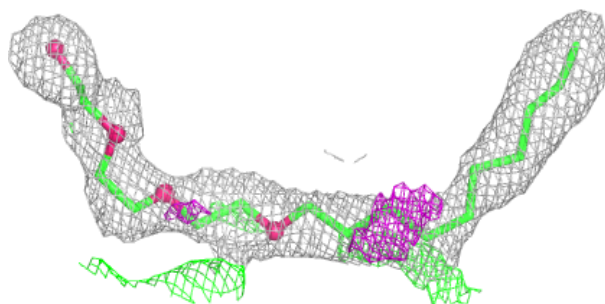


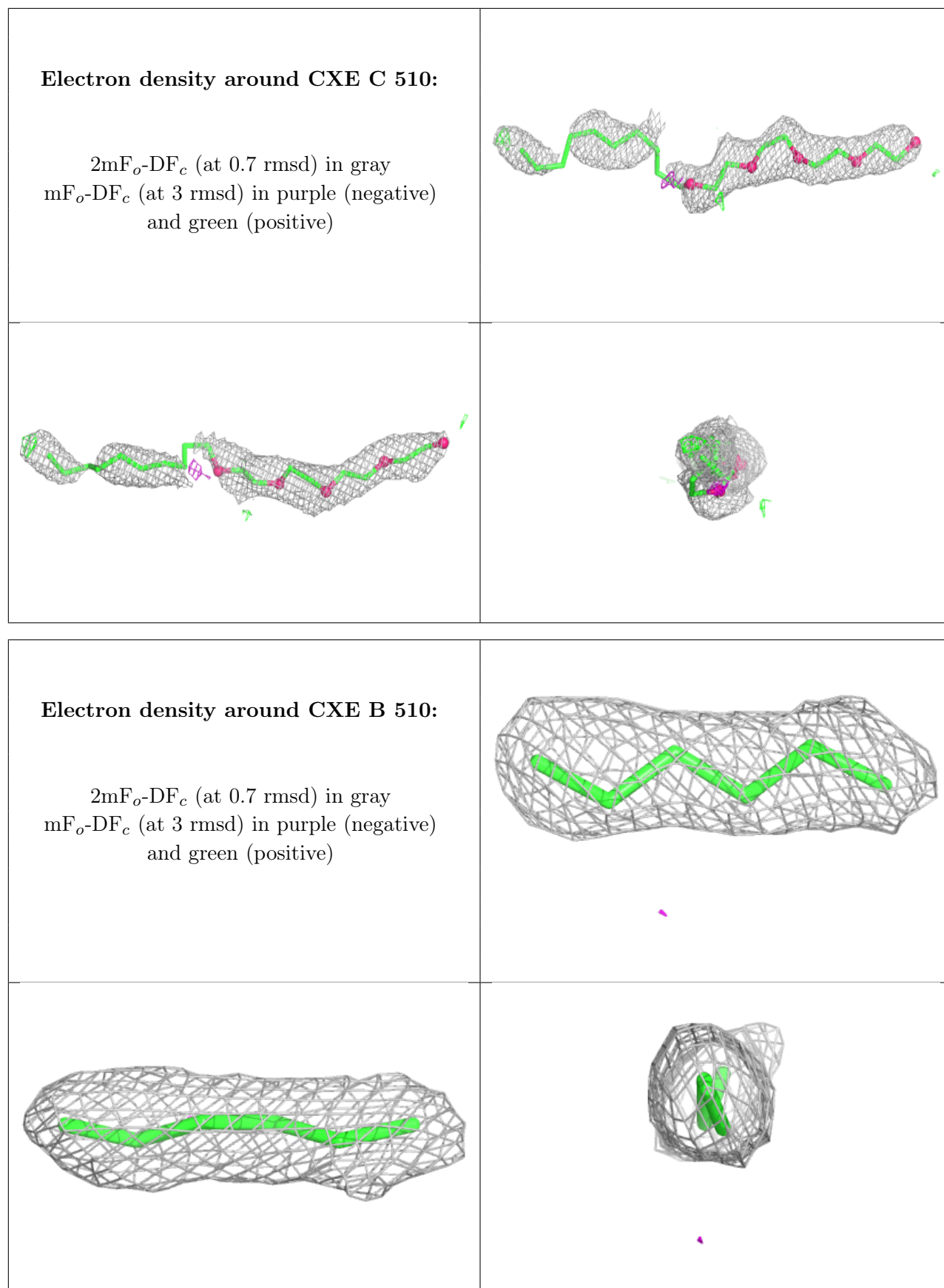
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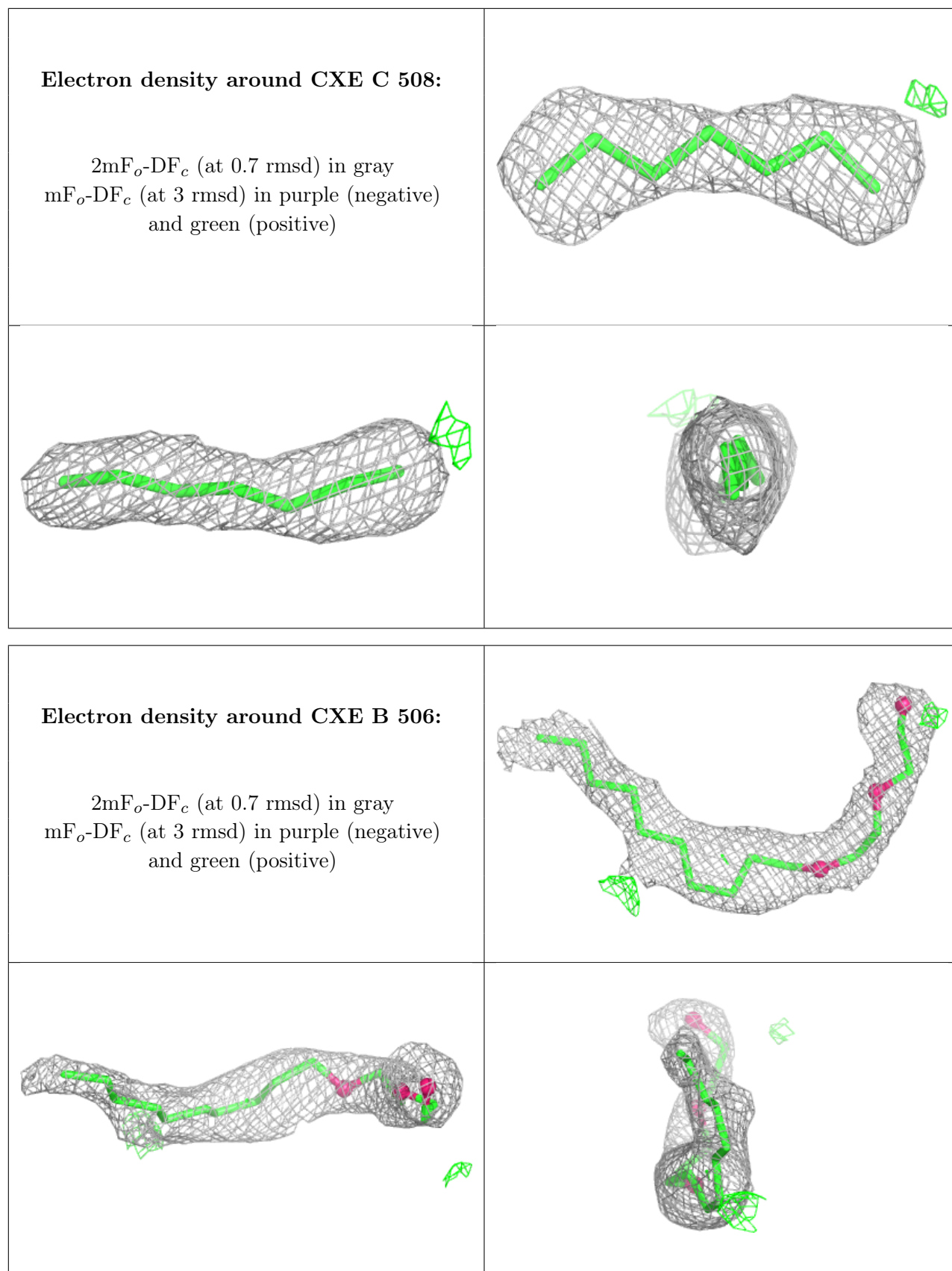
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and green (positive)

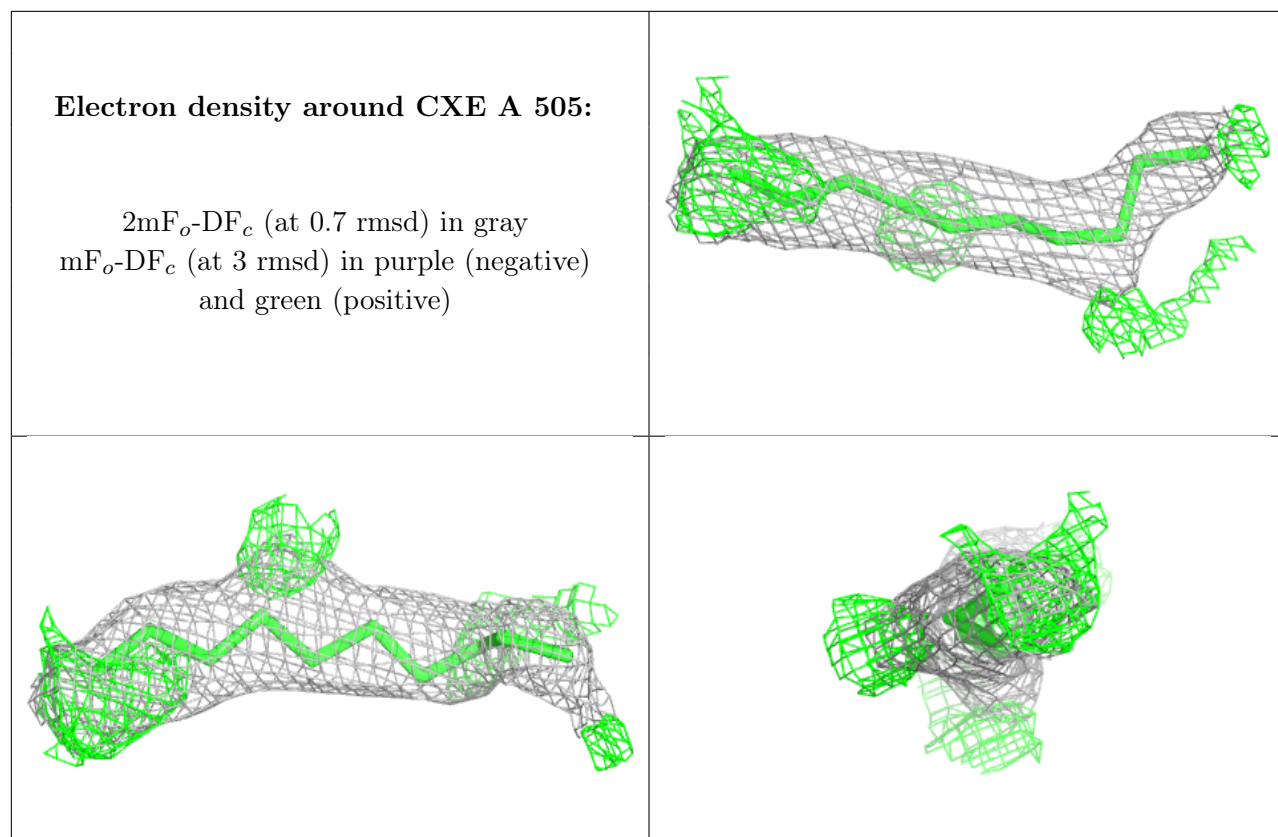
**Electron density around CXE B 502:**

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and green (positive)



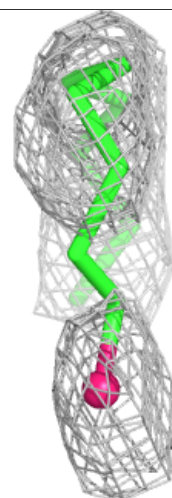
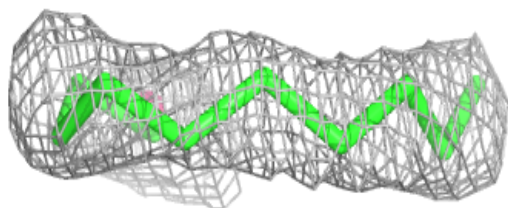
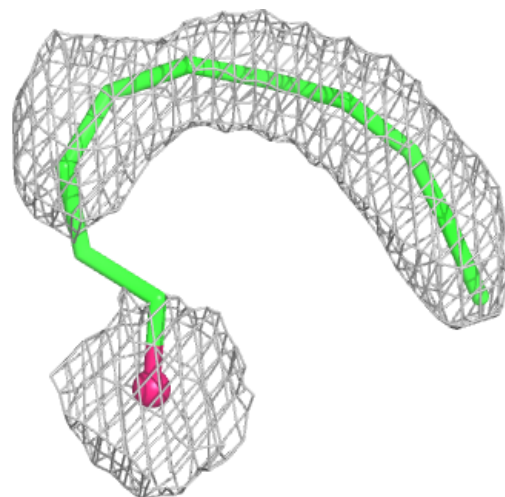


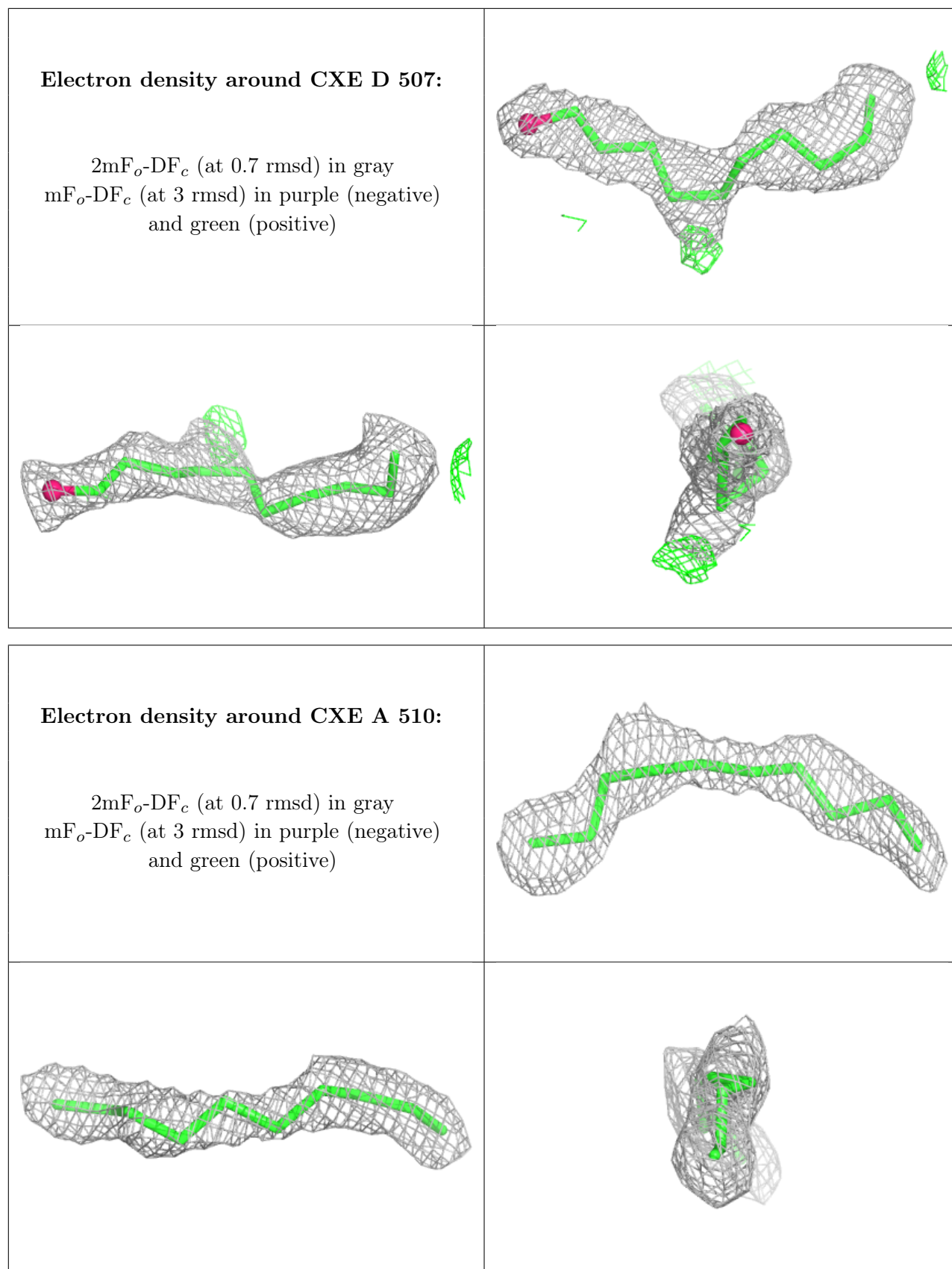




**Electron density around CXE D 506:**

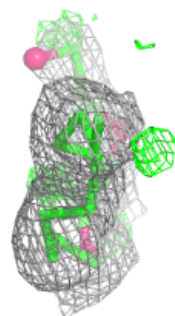
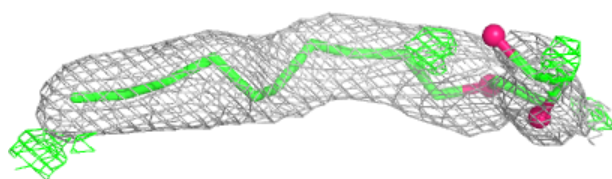
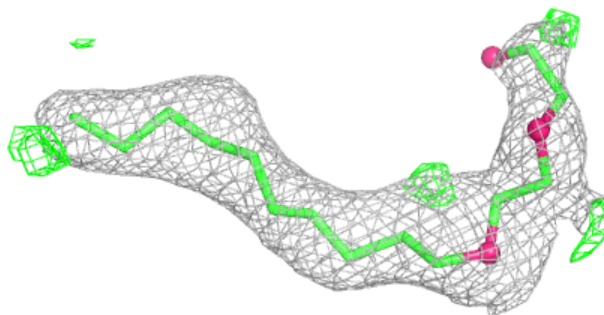
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and green (positive)



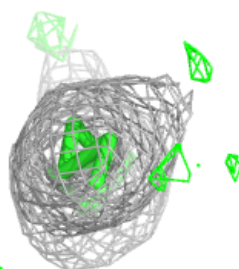
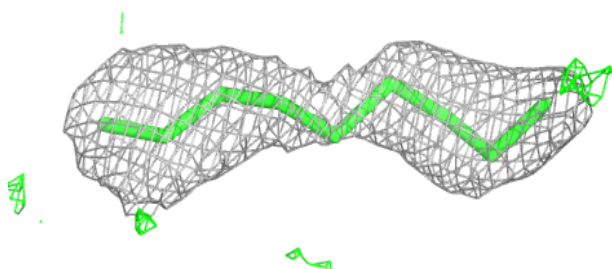
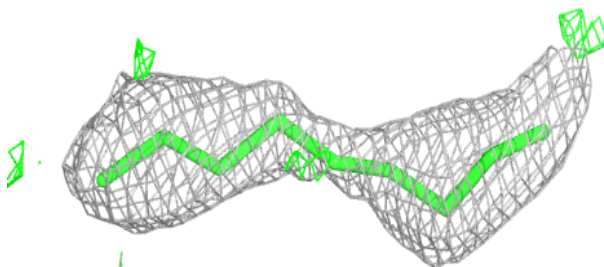


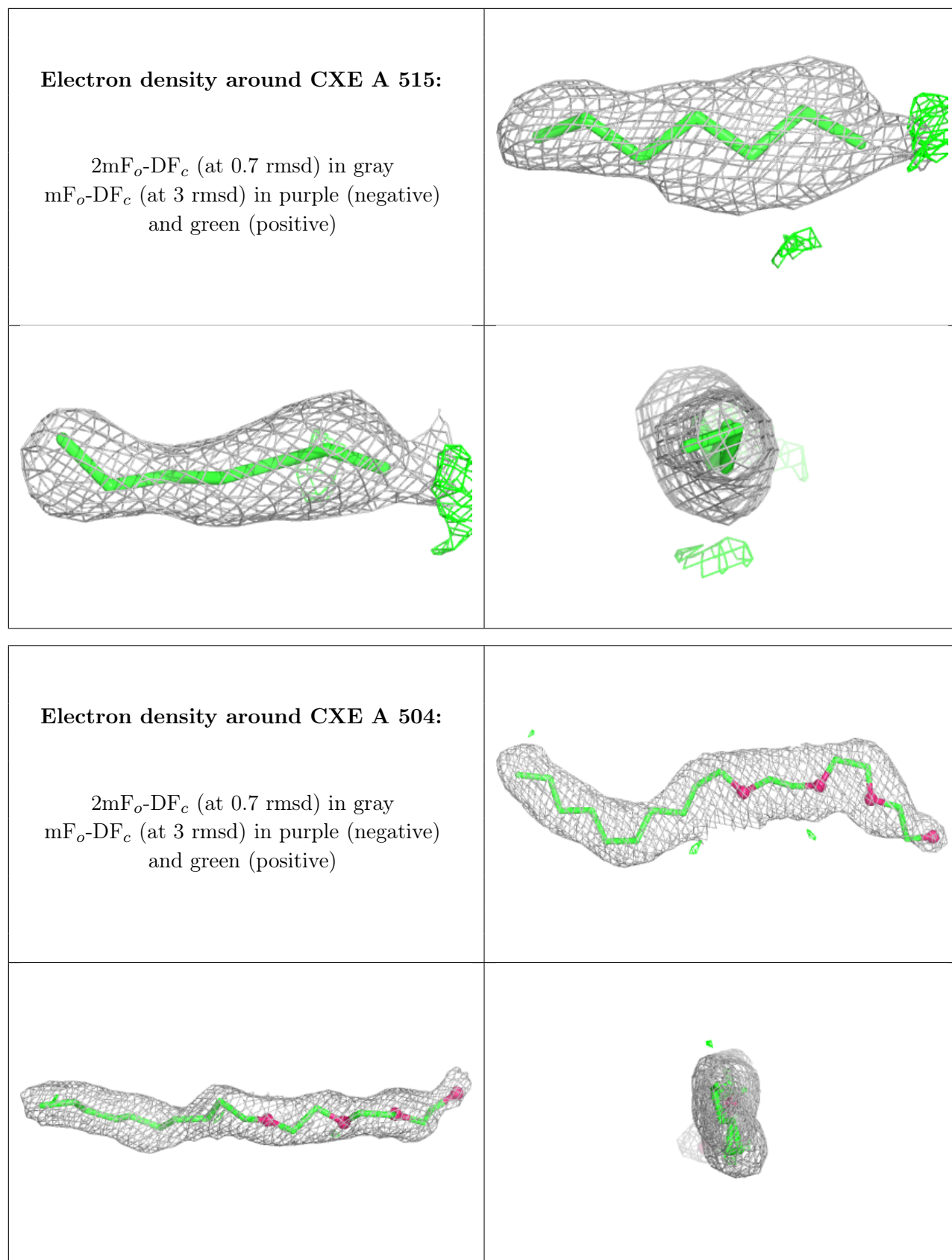
**Electron density around CXE B 503:**

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**Electron density around CXE B 512:**

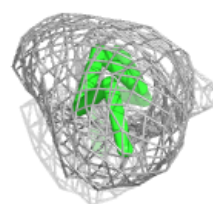
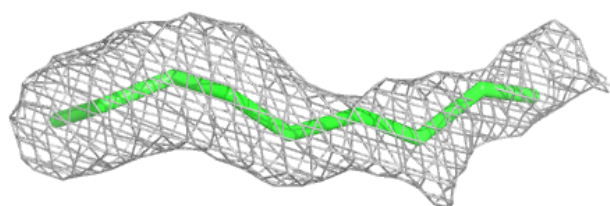
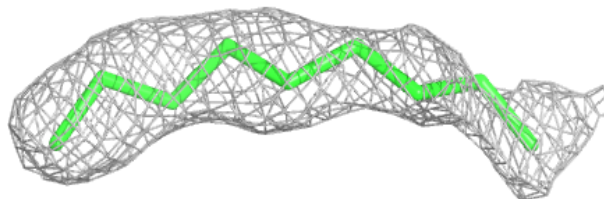
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and green (positive)



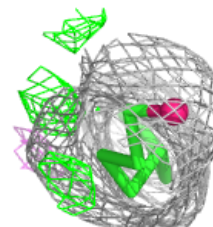
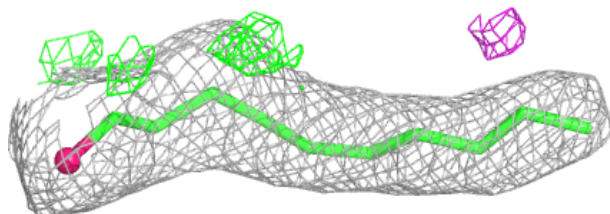
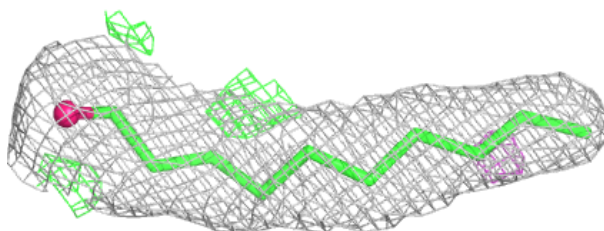


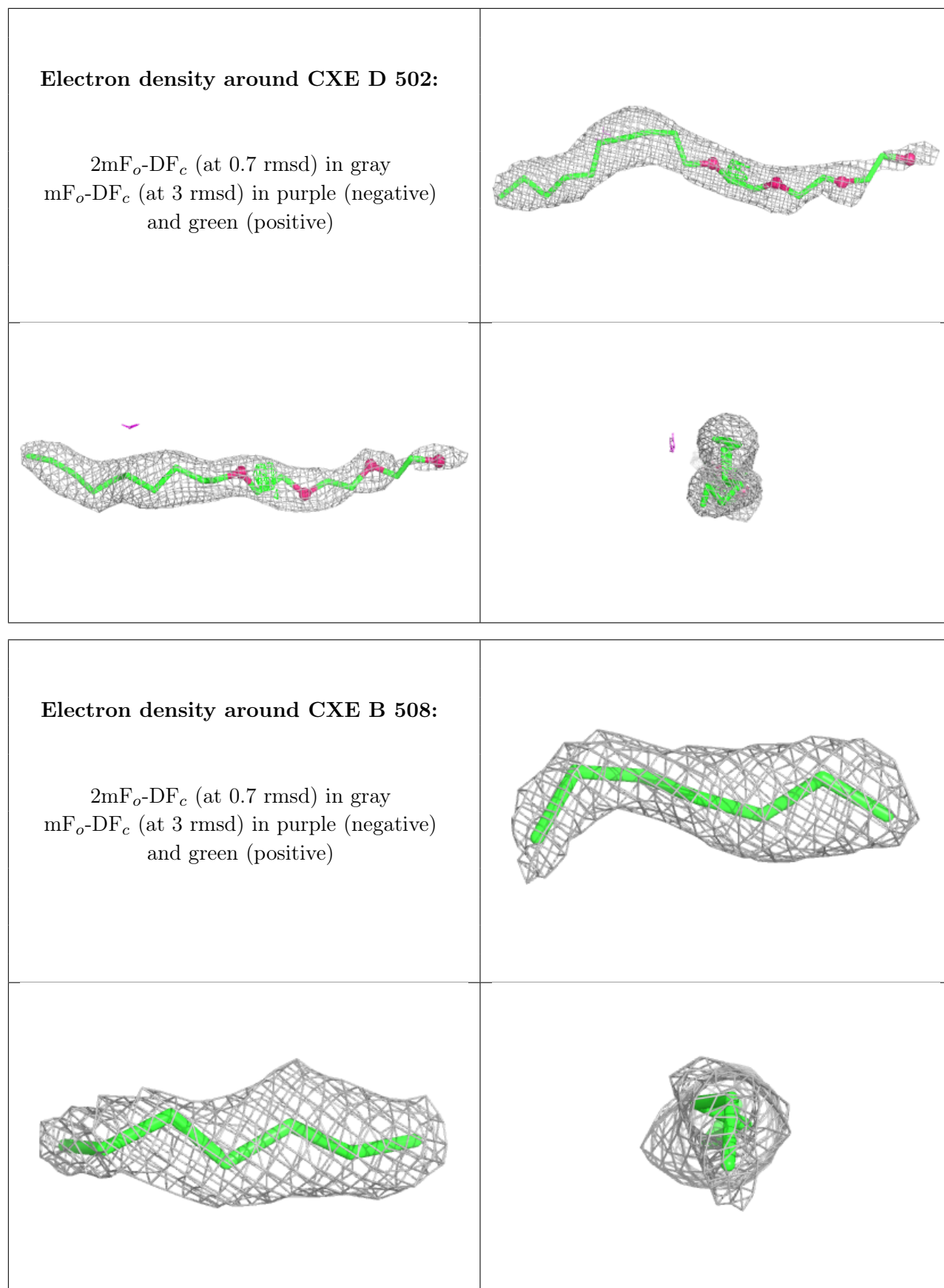
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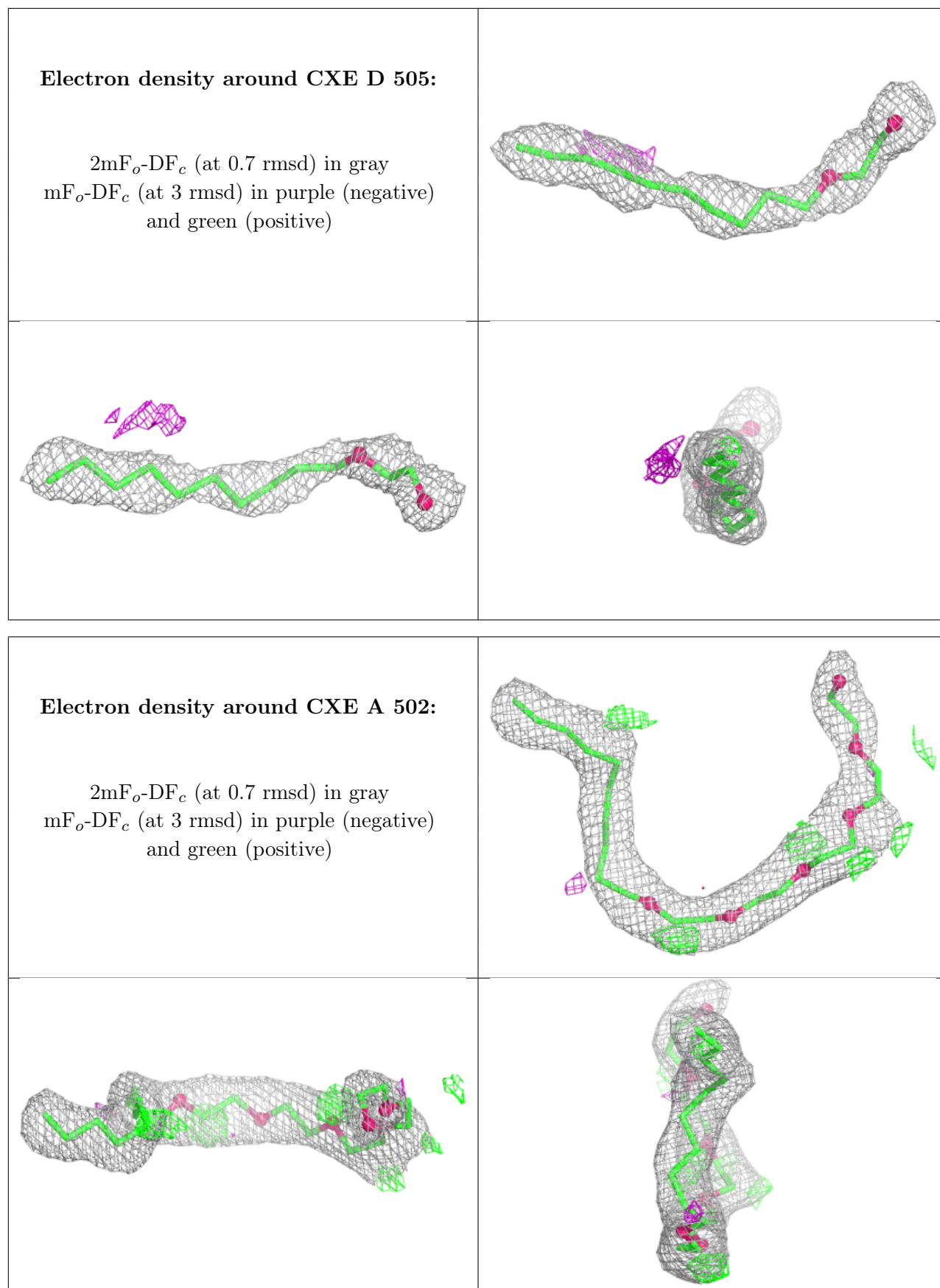
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and green (positive)

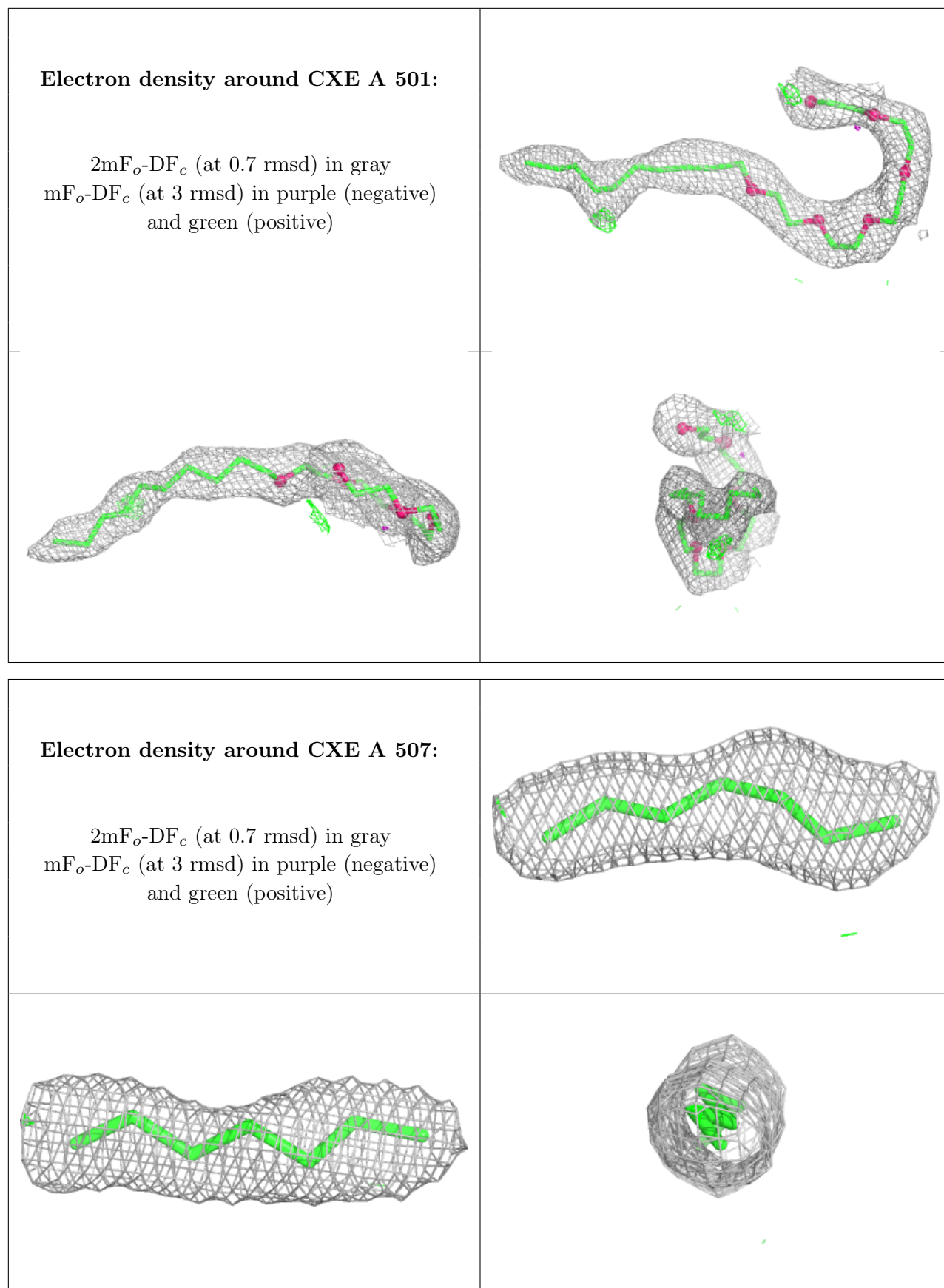
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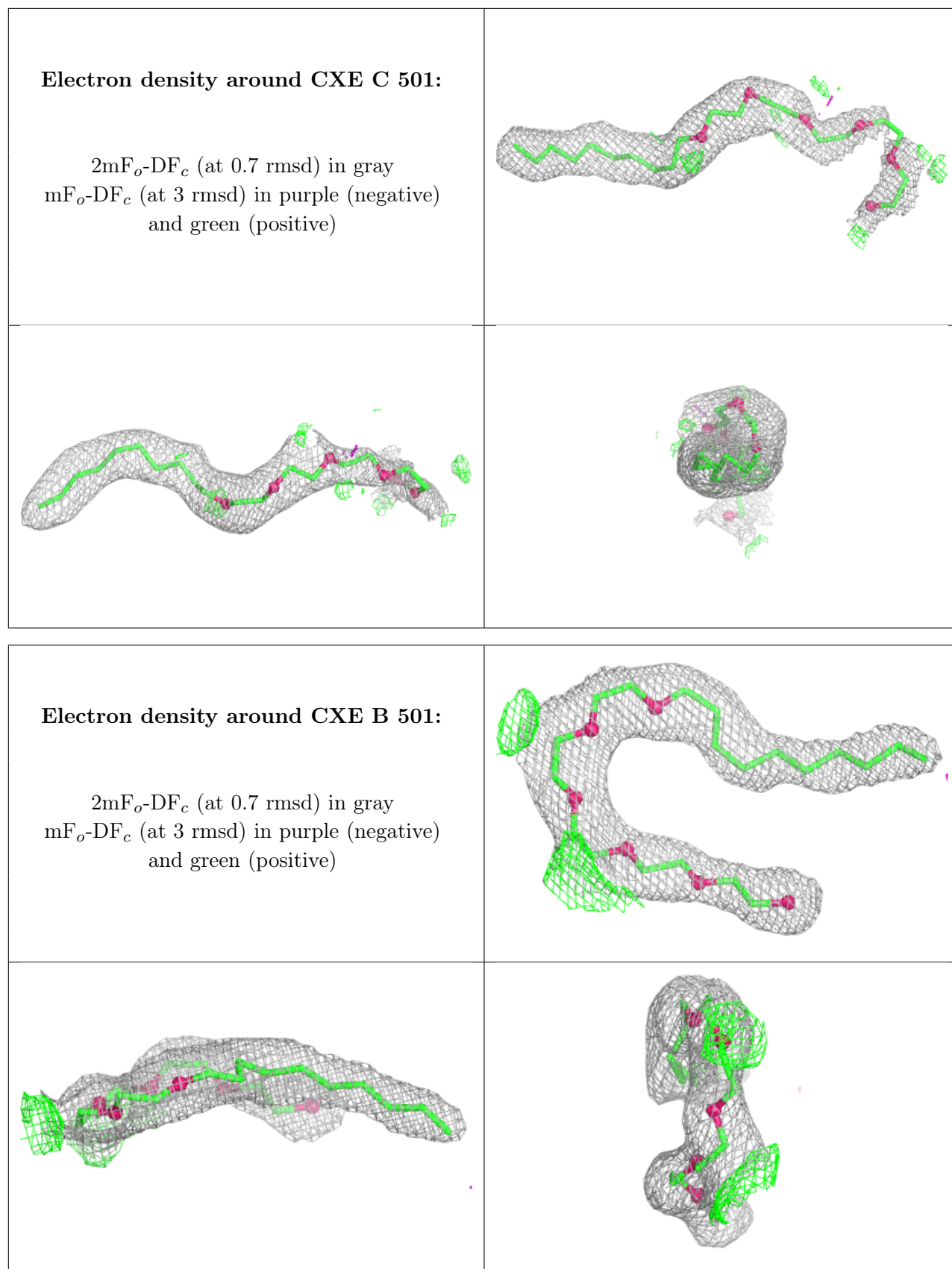
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and green (positive)





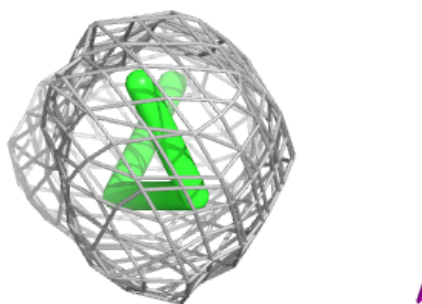
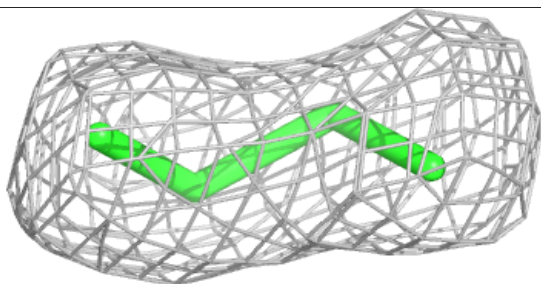
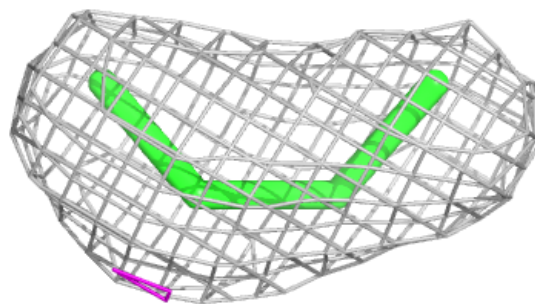




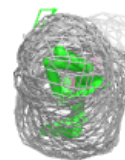
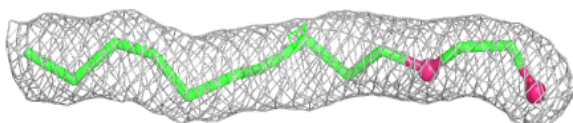
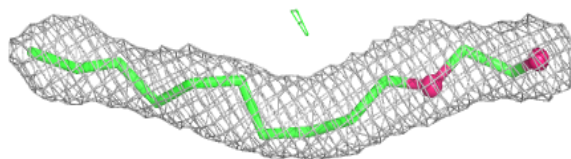


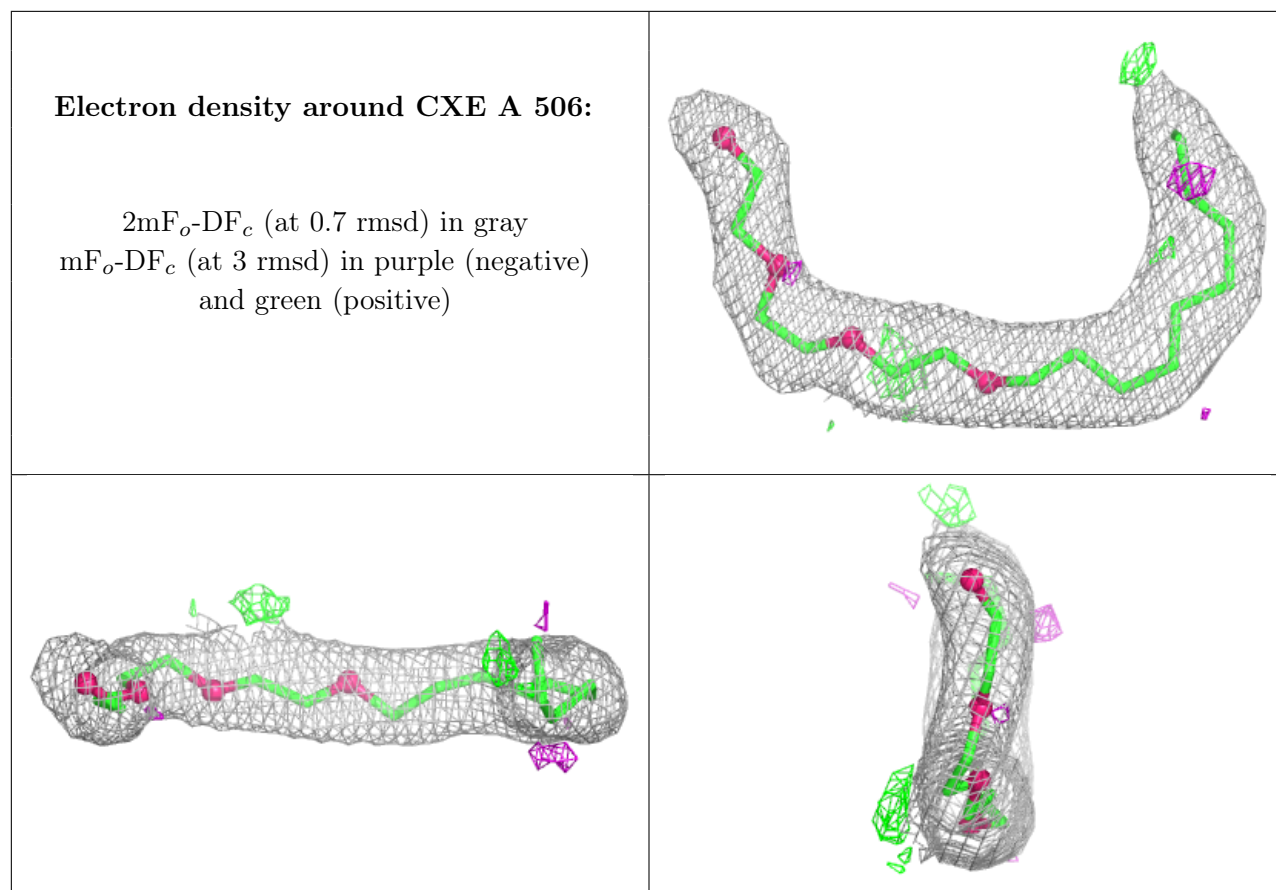
**Electron density around CXE C 515:**

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

**Electron density around CXE D 503:**

$2mF_o-DF_c$  (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.