



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:39 am BST

PDB ID : 4MLB
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

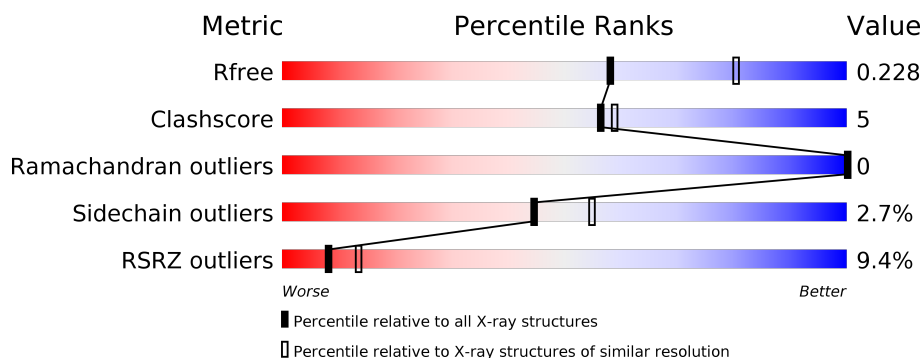
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	492	<div> <div>9%</div> <div>82%</div> <div>9%</div> <div>8%</div> </div>
1	B	492	<div> <div>6%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
1	C	492	<div> <div>9%</div> <div>81%</div> <div>9%</div> <div>8%</div> </div>
1	D	492	<div> <div>11%</div> <div>81%</div> <div>11%</div> <div>8%</div> </div>

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

ria:

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

2 Entry composition

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
1	A	453	Total	C	N	O	S	0	1	0
			3412	2237	557	597	21			
1	B	454	Total	C	N	O	S	0	0	0
			3413	2237	555	600	21			
1	C	452	Total	C	N	O	S	0	2	0
			3418	2241	559	597	21			
1	D	452	Total	C	N	O	S	0	2	0
			3418	2241	559	597	21			

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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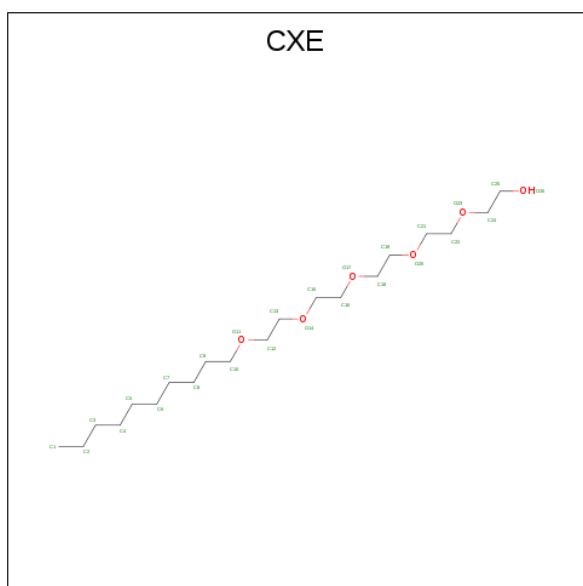
Chain	Residue	Modelled	Actual	Comment	Reference
B	485	HIS	-	EXPRESSION TAG	UNP Q8U2X0
C	-6	MET	-	EXPRESSION TAG	UNP Q8U2X0
C	-5	GLY	-	EXPRESSION TAG	UNP Q8U2X0
C	-4	GLY	-	EXPRESSION TAG	UNP Q8U2X0
C	-3	SER	-	EXPRESSION TAG	UNP Q8U2X0
C	-2	GLU	-	EXPRESSION TAG	UNP Q8U2X0
C	-1	ILE	-	EXPRESSION TAG	UNP 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 (three-letter code: CXE) (formula: $C_{20}H_{42}O_6$).



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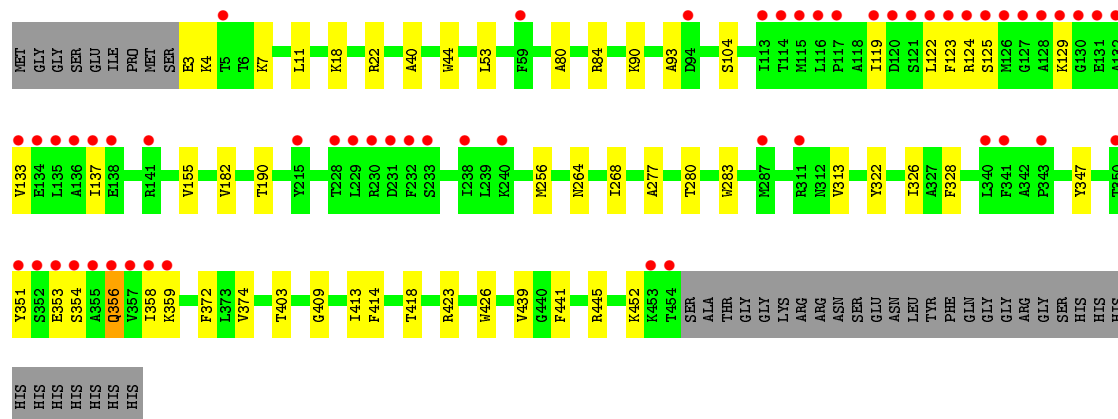
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C 4 4	0	0
2	C	1	Total C 7 7	0	0
2	D	1	Total C O 11 10 1	0	0
2	D	1	Total C O 20 16 4	0	0
2	D	1	Total C O 14 12 2	0	0
2	D	1	Total C 10 10	0	0
2	D	1	Total C O 14 12 2	0	0
2	D	1	Total C O 11 10 1	0	0
2	D	1	Total C O 11 10 1	0	0
2	D	1	Total C 5 5	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: 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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	219.56 Å 94.55 Å 138.82 Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.34 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.203 , 0.231 0.198 , 0.228	Depositor DCC
R_{free} test set	4737 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14749	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CXE, CL

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	0.25	0/3476	0.43	0/4714
1	B	0.23	0/3474	0.40	0/4712
1	C	0.25	0/3485	0.43	0/4725
1	D	0.24	0/3485	0.43	0/4725
All	All	0.24	0/13920	0.42	0/18876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3412	0	3601	33	0
1	B	3413	0	3594	26	0
1	C	3418	0	3610	40	0
1	D	3418	0	3610	33	0
2	A	246	0	420	21	0
2	B	144	0	253	11	0
2	C	273	0	450	23	0
2	D	96	0	174	8	0
3	A	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	152	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 5.

All (152) 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:HG2	1:C:445:ARG:HH11	1.51	0.76
1:A:349:PHE:H	1:A:349:PHE:HD2	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:503:CXE:H071	2:D:505:CXE:H072	1.87	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:C:278:VAL:HG13	1:C:362:LEU:HD21	1.88	0.56
2:B:502:CXE:H021	2:C:505:CXE:H051	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: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:203:LEU:HA	1:A:206:MET:HE2	1.93	0.49
1:A:64:MET:HB3	2:A:513:CXE:H101	1.94	0.49
1:A:344:GLN:OE1	1:A:344:GLN:N	2.45	0.49
2:C:505:CXE:H121	2:C:514:CXE:H013	1.94	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
1:B:337:PHE:CZ	2:B:506:CXE:H032	2.46	0.48
2:A:505:CXE:H032	2:B:511:CXE:H022	1.95	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:H062	2:C:513:CXE:H091	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:C:296:MET:HG3	1:C:327:ALA:HB2	1.97	0.46
2:B:502:CXE:H092	2:C:505:CXE:H152	1.96	0.46
1:D:277:ALA:HB3	1:D:358:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H242	2:C:504:CXE:H212	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:282:ALA:HA	1:C:285:ILE:HD12	1.99	0.45
1:C:59:PHE:CZ	1:C:63:PHE:HB2	2.52	0.45
1:A:378:PHE:CE2	2:A:507:CXE:H022	2.52	0.45
1:C:445:ARG:CG	1:C:445:ARG:HH11	2.25	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:HE3	1:C:129:LYS:HB2	1.89	0.44
1:D:3:GLU:HA	1:D:90:LYS:HE3	1.99	0.44
1:D:7:LYS:HA	1:D:7:LYS:HD2	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:C:344:GLN:NE2	2:C:513:CXE:H212	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:313:VAL:HG11	1:D:452:LYS:HG3	2.00	0.42
1:D:80:ALA:O	1:D:84:ARG:HG2	2.19	0.42
1:A:129:LYS:HD2	1:A:129:LYS:HA	1.92	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:C:214:ALA:HB1	2:C:503:CXE:H181	2.01	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:HD2	1:B:447:ARG:HA	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:H192	2:C:503:CXE:H162	1.34	0.41
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:280:THR:HA	1:D:283:TRP:CD1	2.56	0.41
1:D:84:ARG:HB2	1:D:93:ALA:HB2	2.03	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:HE3	1:D:18:LYS:HB2	1.81	0.41
1:D:356:GLN:NE2	1:D:359:LYS:HD2	2.30	0.41
1:D:256:MET:HG2	1:D:403:THR:HG21	2.02	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: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: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
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%)	343 (96%)	15 (4%)	30	37
1	B	358/389 (92%)	356 (99%)	2 (1%)	86	92
1	C	359/389 (92%)	347 (97%)	12 (3%)	38	46
1	D	359/389 (92%)	350 (98%)	9 (2%)	47	58
All	All	1434/1556 (92%)	1396 (97%)	38 (3%)	44	56

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	184	ASP
1	A	230	ARG
1	A	243	LEU
1	A	288	LEU
1	A	293	ILE
1	A	347	TYR
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	383	SER
1	A	433	ASN
1	B	184	ASP
1	B	226	ASP
1	C	53	LEU
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	372	PHE
1	C	415	VAL
1	C	445	ARG
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	353	GLU
1	D	356	GLN
1	D	372	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	GLN

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Mol	Chain	Res	Type
1	A	407	GLN
1	A	433	ASN
1	B	167	ASN
1	B	407	GLN
1	B	433	ASN
1	C	407	GLN
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 carbohydrates 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	A	512	-	5,5,25	0.25	0	4,4,24	0.40	0
2	CXE	D	502	-	19,19,25	0.29	0	18,18,24	0.58	0
2	CXE	B	509	-	5,5,25	0.25	0	4,4,24	0.35	0
2	CXE	B	507	-	8,8,25	0.21	0	7,7,24	0.60	0
2	CXE	A	503	-	25,25,25	0.33	0	24,24,24	0.68	0
2	CXE	C	507	-	9,9,25	0.25	0	8,8,24	0.49	0
2	CXE	A	504	-	19,19,25	0.31	0	18,18,24	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CXE	D	506	-	10,10,25	0.25	0	9,9,24	0.50	0
2	CXE	B	511	-	5,5,25	0.25	0	4,4,24	0.40	0
2	CXE	A	510	-	9,9,25	0.23	0	8,8,24	0.55	0
2	CXE	D	501	-	10,10,25	0.21	0	9,9,24	0.58	0
2	CXE	C	501	-	25,25,25	0.40	0	24,24,24	0.44	0
2	CXE	B	505	-	9,9,25	0.24	0	8,8,24	0.55	0
2	CXE	A	516	-	6,6,25	0.21	0	5,5,24	0.62	0
2	CXE	C	511	-	9,9,25	0.23	0	8,8,24	0.56	0
2	CXE	A	506	-	19,19,25	0.31	0	18,18,24	0.56	0
2	CXE	C	502	-	25,25,25	0.37	0	24,24,24	0.58	0
2	CXE	C	512	-	15,15,25	0.44	0	14,14,24	0.44	0
2	CXE	A	502	-	25,25,25	0.40	0	24,24,24	0.43	0
2	CXE	D	503	-	13,13,25	0.31	0	12,12,24	0.49	0
2	CXE	B	503	-	16,16,25	0.33	0	15,15,24	0.59	0
2	CXE	B	504	-	10,10,25	0.25	0	9,9,24	0.50	0
2	CXE	D	507	-	10,10,25	0.24	0	9,9,24	0.51	0
2	CXE	C	503	-	25,25,25	0.39	0	24,24,24	0.60	0
2	CXE	C	509	-	16,16,25	0.37	0	15,15,24	0.57	0
2	CXE	C	513	-	22,22,25	0.35	0	21,21,24	0.66	0
2	CXE	A	505	-	9,9,25	0.18	0	8,8,24	0.83	0
2	CXE	D	505	-	13,13,25	0.27	0	12,12,24	0.50	0
2	CXE	B	510	-	5,5,25	0.23	0	4,4,24	0.41	0
2	CXE	A	514	-	8,8,25	0.24	0	7,7,24	0.52	0
2	CXE	C	510	-	22,22,25	0.37	0	21,21,24	0.50	0
2	CXE	A	508	-	13,13,25	0.29	0	12,12,24	0.52	0
2	CXE	C	508	-	6,6,25	0.23	0	5,5,24	0.52	0
2	CXE	A	513	-	19,19,25	0.32	0	18,18,24	0.53	0
2	CXE	B	506	-	16,16,25	0.36	0	15,15,24	0.52	0
2	CXE	A	517	-	4,4,25	0.22	0	3,3,24	0.50	0
2	CXE	A	507	-	6,6,25	0.24	0	5,5,24	0.41	0
2	CXE	B	502	-	19,19,25	0.42	0	18,18,24	0.47	0
2	CXE	C	516	-	6,6,25	0.26	0	5,5,24	0.49	0
2	CXE	B	512	-	8,8,25	0.26	0	7,7,24	0.45	0
2	CXE	B	501	-	25,25,25	0.39	0	24,24,24	0.45	0
2	CXE	A	501	-	25,25,25	0.40	0	24,24,24	0.51	0
2	CXE	C	506	-	14,14,25	0.33	0	13,13,24	0.54	0
2	CXE	A	511	-	9,9,25	0.23	0	8,8,24	0.57	0
2	CXE	C	515	-	3,3,25	0.35	0	2,2,24	0.61	0
2	CXE	C	505	-	19,19,25	0.38	0	18,18,24	0.75	0
2	CXE	A	515	-	6,6,25	0.24	0	5,5,24	0.42	0
2	CXE	D	504	-	9,9,25	0.22	0	8,8,24	0.62	0
2	CXE	B	508	-	6,6,25	0.25	0	5,5,24	0.41	0
2	CXE	D	508	-	4,4,25	0.24	0	3,3,24	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CXE	C	514	-	16,16,25	0.34	0	15,15,24	0.46	0
2	CXE	C	504	-	25,25,25	0.40	0	24,24,24	0.48	0
2	CXE	A	509	-	22,22,25	0.38	0	21,21,24	0.40	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	A	512	-	-	0/3/3/23	-
2	CXE	D	502	-	-	11/17/17/23	-
2	CXE	B	509	-	-	1/3/3/23	-
2	CXE	B	507	-	-	3/6/6/23	-
2	CXE	A	503	-	-	10/23/23/23	-
2	CXE	C	507	-	-	3/7/7/23	-
2	CXE	A	504	-	-	8/17/17/23	-
2	CXE	D	506	-	-	6/8/8/23	-
2	CXE	B	511	-	-	2/3/3/23	-
2	CXE	A	510	-	-	3/7/7/23	-
2	CXE	D	501	-	-	2/8/8/23	-
2	CXE	C	501	-	-	10/23/23/23	-
2	CXE	B	505	-	-	0/7/7/23	-
2	CXE	A	516	-	-	2/4/4/23	-
2	CXE	C	511	-	-	0/7/7/23	-
2	CXE	A	506	-	-	8/17/17/23	-
2	CXE	C	502	-	-	13/23/23/23	-
2	CXE	C	512	-	-	8/13/13/23	-
2	CXE	A	502	-	-	3/23/23/23	-
2	CXE	D	503	-	-	7/11/11/23	-
2	CXE	B	503	-	-	10/14/14/23	-
2	CXE	B	504	-	-	0/8/8/23	-
2	CXE	D	507	-	-	4/8/8/23	-
2	CXE	C	503	-	-	12/23/23/23	-
2	CXE	C	509	-	-	8/14/14/23	-
2	CXE	C	513	-	-	12/20/20/23	-
2	CXE	A	505	-	-	3/7/7/23	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CXE	D	505	-	-	3/11/11/23	-
2	CXE	B	510	-	-	1/3/3/23	-
2	CXE	A	514	-	-	3/6/6/23	-
2	CXE	C	510	-	-	8/20/20/23	-
2	CXE	A	508	-	-	9/11/11/23	-
2	CXE	C	508	-	-	1/4/4/23	-
2	CXE	A	513	-	-	7/17/17/23	-
2	CXE	B	506	-	-	6/14/14/23	-
2	CXE	A	517	-	-	2/2/2/23	-
2	CXE	A	507	-	-	2/4/4/23	-
2	CXE	B	502	-	-	6/17/17/23	-
2	CXE	C	516	-	-	3/4/4/23	-
2	CXE	B	512	-	-	4/6/6/23	-
2	CXE	B	501	-	-	1/23/23/23	-
2	CXE	A	501	-	-	7/23/23/23	-
2	CXE	C	506	-	-	9/12/12/23	-
2	CXE	A	511	-	-	2/7/7/23	-
2	CXE	C	515	-	-	0/1/1/23	-
2	CXE	C	505	-	-	9/17/17/23	-
2	CXE	A	515	-	-	2/4/4/23	-
2	CXE	D	504	-	-	2/7/7/23	-
2	CXE	B	508	-	-	2/4/4/23	-
2	CXE	D	508	-	-	0/2/2/23	-
2	CXE	C	514	-	-	3/14/14/23	-
2	CXE	C	504	-	-	13/23/23/23	-
2	CXE	A	509	-	-	3/20/20/23	-

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	C	504	CXE	O23-C24-C25-O26

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

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Mol	Chain	Res	Type	Atoms
2	C	506	CXE	C4-C5-C6-C7
2	D	502	CXE	C5-C6-C7-C8
2	D	502	CXE	O14-C15-C16-O17
2	A	503	CXE	C3-C4-C5-C6
2	C	504	CXE	C19-C18-O17-C16
2	A	510	CXE	C6-C7-C8-C9
2	B	503	CXE	C6-C7-C8-C9
2	C	516	CXE	C2-C3-C4-C5
2	B	512	CXE	C5-C6-C7-C8
2	D	502	CXE	C4-C5-C6-C7
2	A	511	CXE	C4-C5-C6-C7
2	C	502	CXE	O14-C15-C16-O17
2	C	505	CXE	C4-C5-C6-C7
2	C	513	CXE	O20-C21-C22-O23
2	A	504	CXE	O11-C12-C13-O14
2	B	507	CXE	C2-C3-C4-C5
2	A	510	CXE	C5-C6-C7-C8
2	B	508	CXE	C2-C3-C4-C5
2	C	507	CXE	C4-C5-C6-C7
2	D	506	CXE	C6-C7-C8-C9
2	C	505	CXE	C5-C6-C7-C8
2	A	514	CXE	C2-C3-C4-C5
2	C	506	CXE	C5-C6-C7-C8
2	D	502	CXE	C3-C4-C5-C6
2	C	503	CXE	C5-C6-C7-C8
2	C	502	CXE	C7-C8-C9-C10
2	A	504	CXE	C7-C8-C9-C10
2	C	510	CXE	O11-C10-C9-C8
2	A	506	CXE	O17-C18-C19-O20
2	C	512	CXE	O23-C24-C25-O26
2	D	505	CXE	O11-C12-C13-O14
2	A	510	CXE	C2-C3-C4-C5
2	A	506	CXE	C7-C8-C9-C10
2	C	502	CXE	C2-C3-C4-C5
2	B	503	CXE	C2-C3-C4-C5
2	C	506	CXE	C6-C7-C8-C9
2	C	506	CXE	O11-C12-C13-O14
2	A	509	CXE	C3-C4-C5-C6
2	C	505	CXE	O17-C18-C19-O20
2	A	513	CXE	O14-C15-C16-O17
2	A	501	CXE	C5-C6-C7-C8
2	A	516	CXE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	C	509	CXE	C2-C3-C4-C5
2	C	509	CXE	C6-C7-C8-C9
2	A	508	CXE	C5-C6-C7-C8
2	A	503	CXE	C7-C8-C9-C10
2	D	503	CXE	C7-C8-C9-C10
2	D	501	CXE	C4-C5-C6-C7
2	B	502	CXE	C3-C4-C5-C6
2	A	504	CXE	O14-C15-C16-O17
2	B	502	CXE	C2-C3-C4-C5
2	C	513	CXE	C4-C5-C6-C7
2	D	506	CXE	C2-C3-C4-C5
2	C	502	CXE	O23-C24-C25-O26
2	A	513	CXE	O17-C18-C19-O20
2	A	514	CXE	C6-C7-C8-C9
2	C	503	CXE	O20-C21-C22-O23
2	B	511	CXE	C2-C3-C4-C5
2	C	514	CXE	C7-C8-C9-C10
2	C	507	CXE	C1-C2-C3-C4
2	A	514	CXE	C1-C2-C3-C4
2	A	517	CXE	C2-C3-C4-C5
2	B	511	CXE	C3-C4-C5-C6
2	A	508	CXE	C2-C3-C4-C5
2	A	517	CXE	C1-C2-C3-C4
2	A	506	CXE	C6-C7-C8-C9
2	B	503	CXE	C9-C10-O11-C12
2	C	513	CXE	O14-C15-C16-O17
2	B	503	CXE	C3-C4-C5-C6
2	A	505	CXE	C6-C7-C8-C9
2	B	503	CXE	C7-C8-C9-C10
2	C	505	CXE	C3-C4-C5-C6
2	A	509	CXE	C2-C3-C4-C5
2	A	506	CXE	C1-C2-C3-C4
2	D	507	CXE	C4-C5-C6-C7
2	B	512	CXE	C2-C3-C4-C5
2	C	504	CXE	O17-C18-C19-O20
2	C	503	CXE	O11-C12-C13-O14
2	D	506	CXE	C7-C8-C9-C10
2	A	511	CXE	C3-C4-C5-C6
2	A	515	CXE	C1-C2-C3-C4
2	C	506	CXE	C7-C8-C9-C10
2	C	501	CXE	O17-C18-C19-O20
2	C	516	CXE	C4-C5-C6-C7

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

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

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Mol	Chain	Res	Type	Atoms
2	C	503	CXE	C25-C24-O23-C22
2	C	512	CXE	C22-C21-O20-C19
2	A	513	CXE	C1-C2-C3-C4
2	C	502	CXE	C15-C16-O17-C18
2	C	513	CXE	C15-C16-O17-C18
2	C	503	CXE	C9-C10-O11-C12
2	C	504	CXE	C15-C16-O17-C18
2	A	502	CXE	O14-C15-C16-O17
2	C	502	CXE	O20-C21-C22-O23
2	B	503	CXE	C13-C12-O11-C10
2	A	506	CXE	O11-C12-C13-O14
2	C	503	CXE	O14-C15-C16-O17
2	C	510	CXE	C4-C5-C6-C7
2	C	502	CXE	C6-C7-C8-C9
2	D	503	CXE	C1-C2-C3-C4
2	B	501	CXE	C9-C10-O11-C12
2	A	502	CXE	C4-C5-C6-C7
2	B	503	CXE	C16-C15-O14-C13
2	C	501	CXE	O14-C15-C16-O17
2	C	501	CXE	C13-C12-O11-C10
2	A	505	CXE	C5-C6-C7-C8
2	C	505	CXE	O11-C12-C13-O14
2	A	515	CXE	C4-C5-C6-C7
2	C	512	CXE	O17-C18-C19-O20
2	C	513	CXE	C18-C19-O20-C21
2	C	510	CXE	O14-C15-C16-O17
2	A	516	CXE	C4-C5-C6-C7
2	C	509	CXE	C12-C13-O14-C15
2	A	503	CXE	O17-C18-C19-O20
2	A	503	CXE	C16-C15-O14-C13
2	C	510	CXE	O11-C12-C13-O14
2	D	503	CXE	O11-C12-C13-O14
2	D	507	CXE	C2-C3-C4-C5
2	C	508	CXE	C4-C5-C6-C7
2	D	506	CXE	C3-C4-C5-C6
2	C	505	CXE	C6-C7-C8-C9
2	C	504	CXE	O14-C15-C16-O17
2	B	506	CXE	O14-C15-C16-O17
2	C	502	CXE	C13-C12-O11-C10
2	A	504	CXE	C5-C6-C7-C8
2	C	512	CXE	C19-C18-O17-C16
2	C	504	CXE	O11-C12-C13-O14

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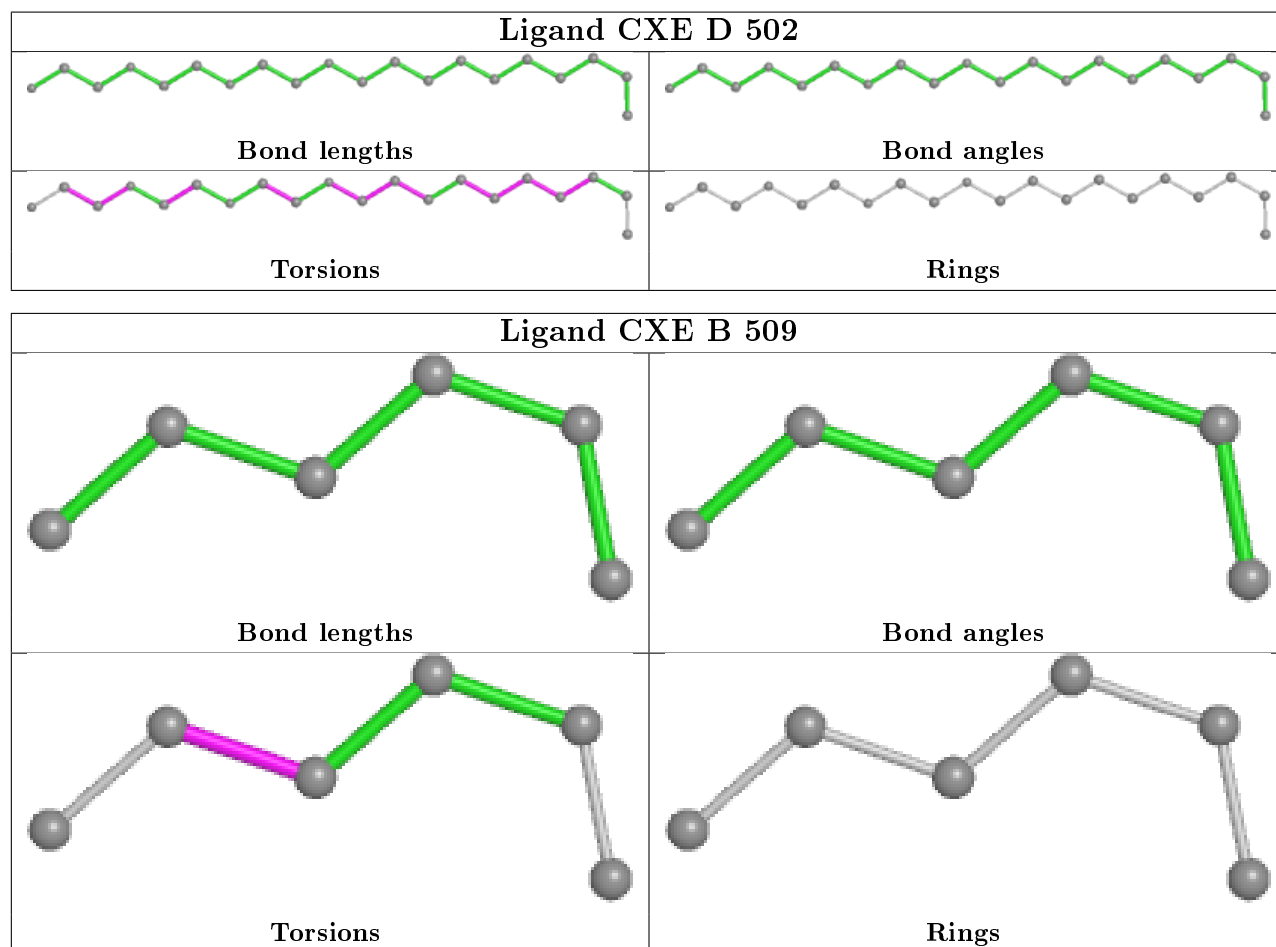
Mol	Chain	Res	Type	Atoms
2	C	510	CXE	O17-C18-C19-O20
2	A	513	CXE	C12-C13-O14-C15

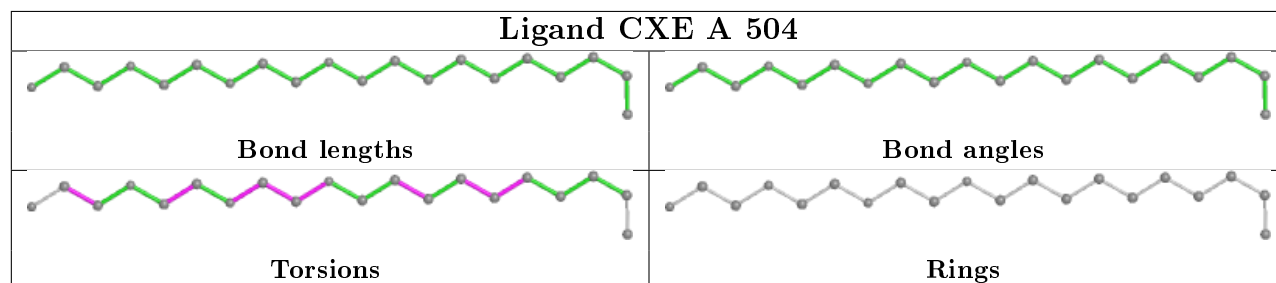
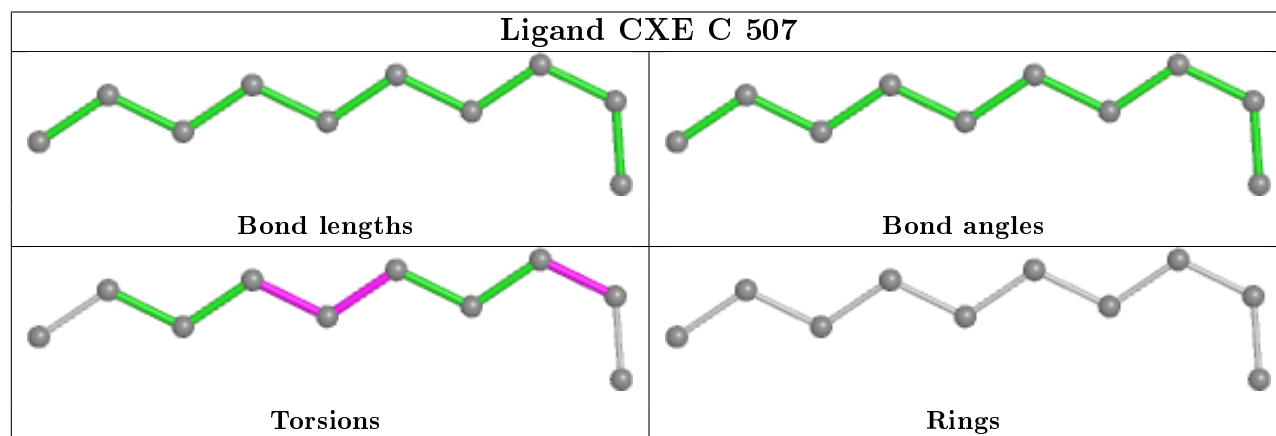
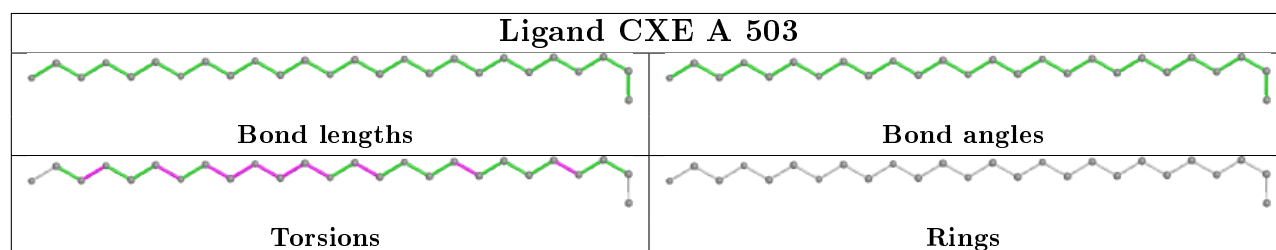
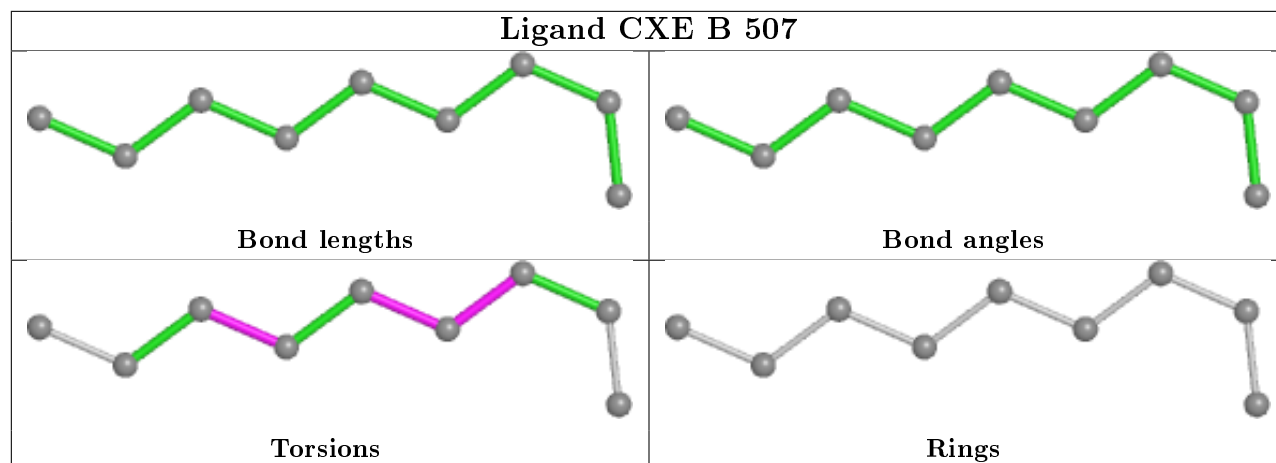
There are no ring outliers.

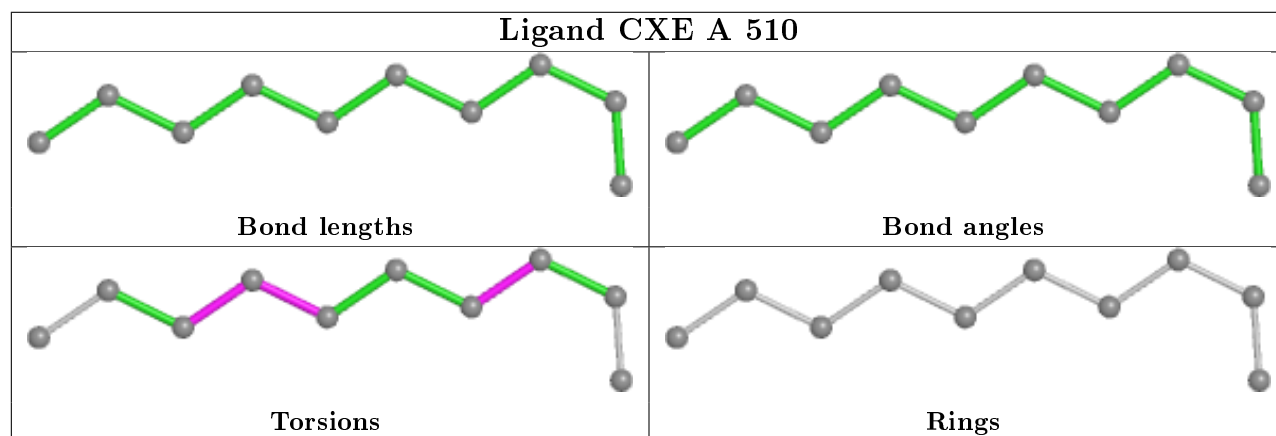
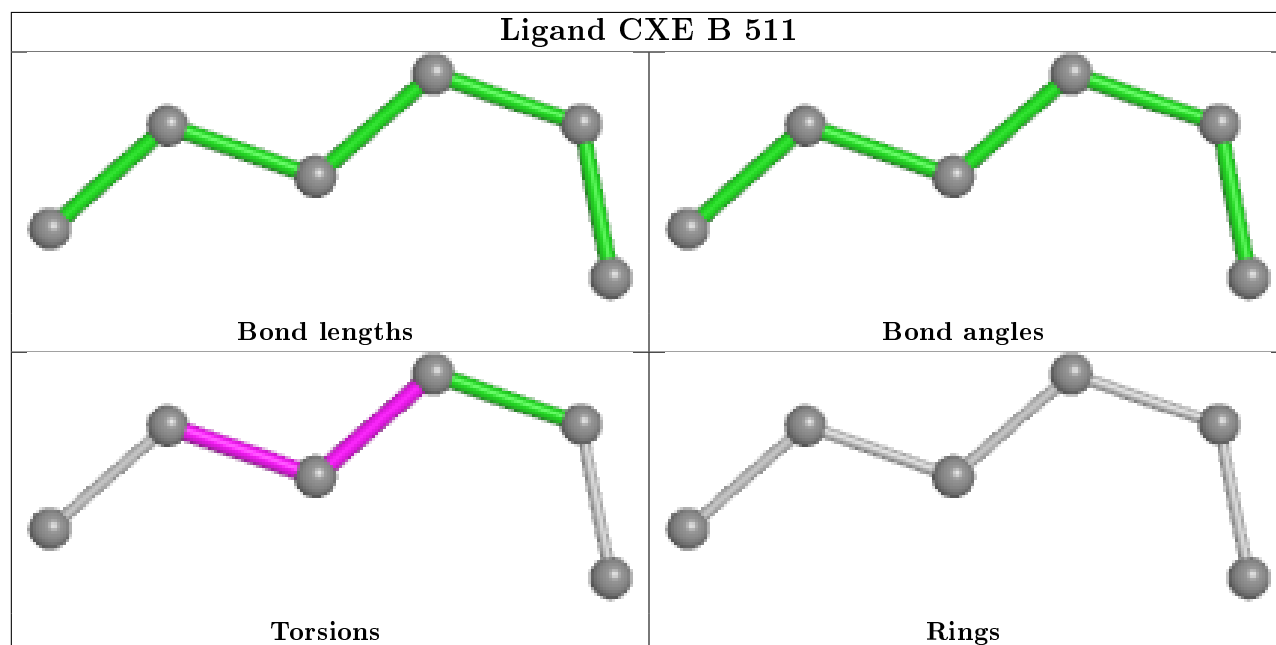
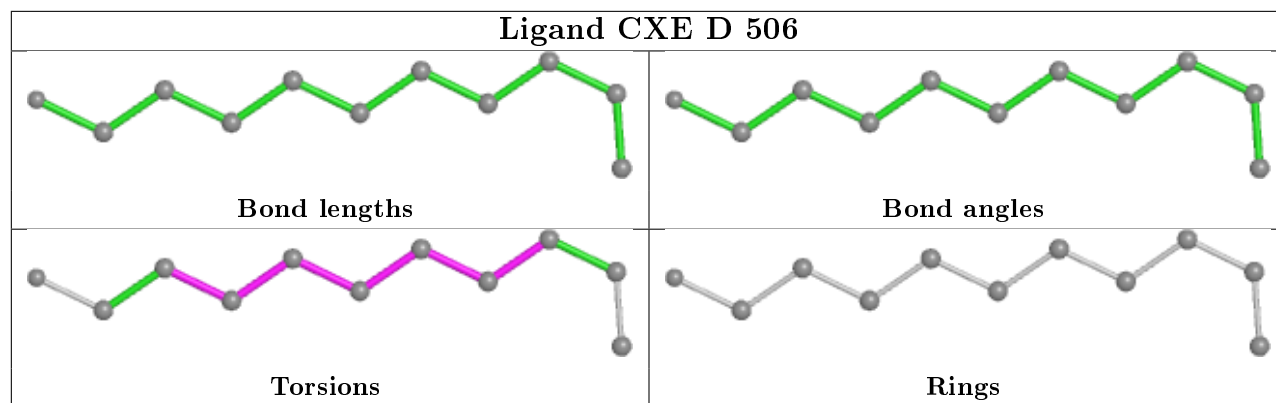
34 monomers are involved in 57 short contacts:

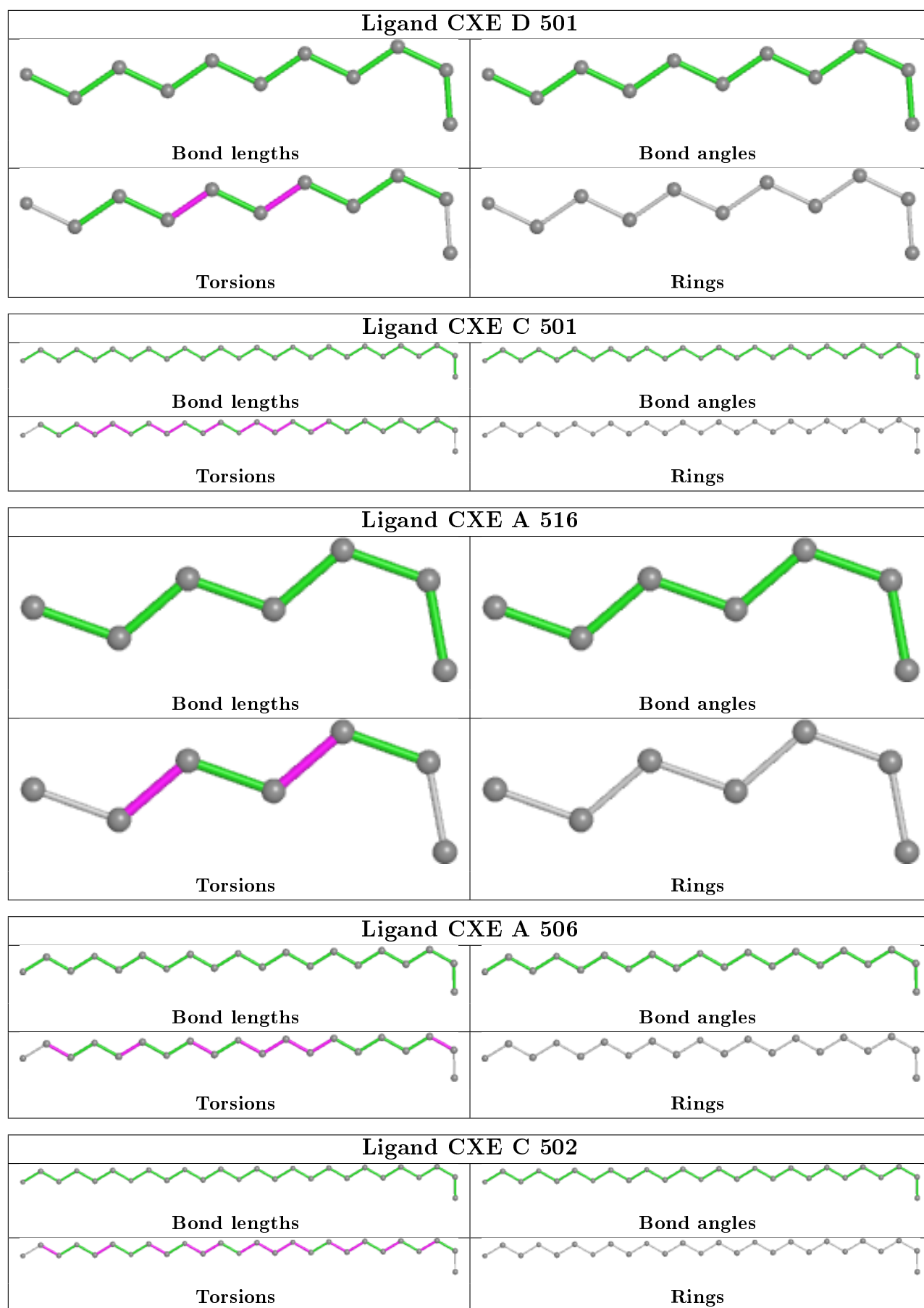
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	502	CXE	1	0
2	A	503	CXE	2	0
2	A	504	CXE	1	0
2	B	511	CXE	1	0
2	D	501	CXE	2	0
2	C	501	CXE	3	0
2	A	516	CXE	1	0
2	C	511	CXE	1	0
2	A	506	CXE	6	0
2	C	502	CXE	1	0
2	C	512	CXE	3	0
2	A	502	CXE	3	0
2	D	503	CXE	1	0
2	B	503	CXE	1	0
2	D	507	CXE	3	0
2	C	503	CXE	4	0
2	C	513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

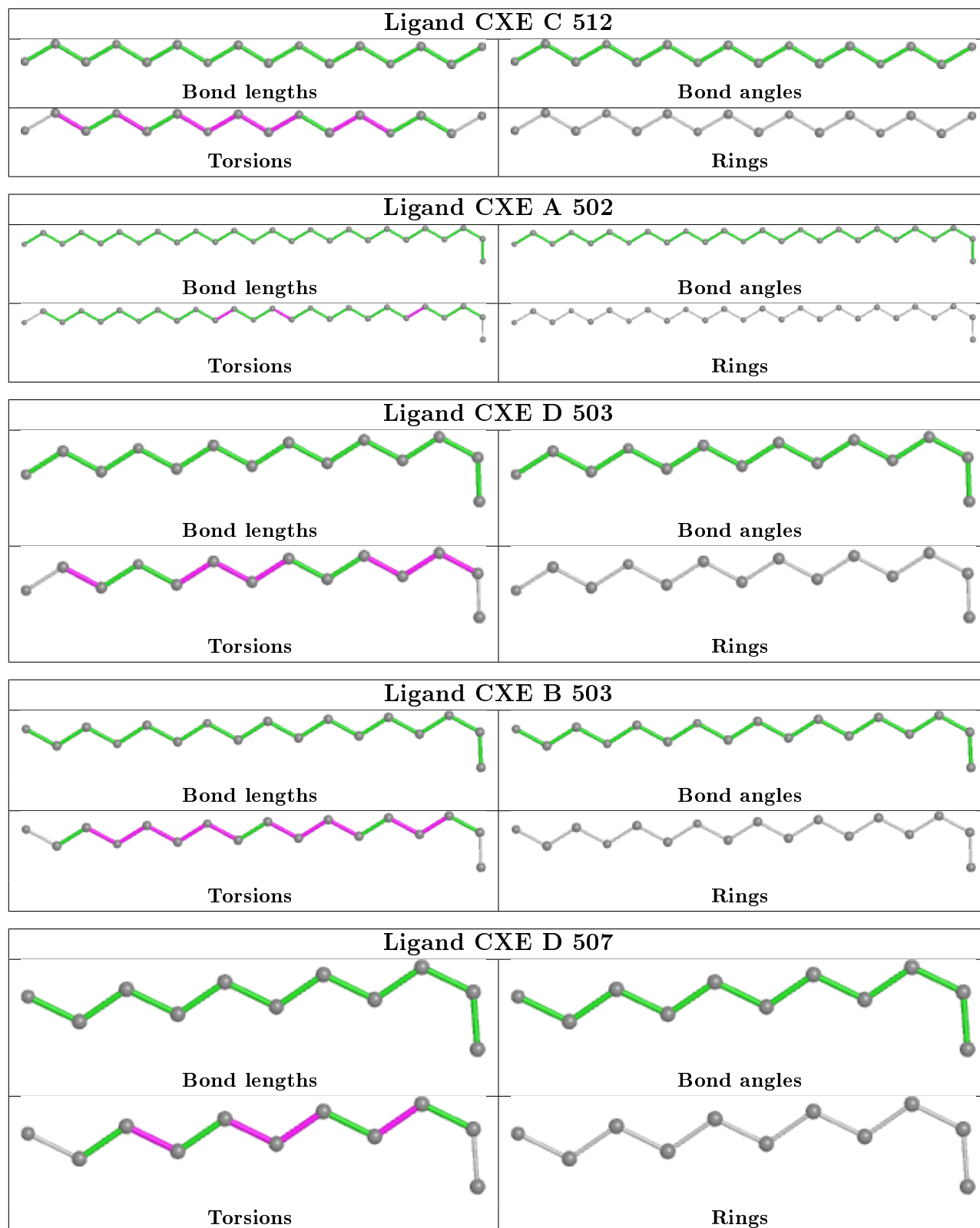
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

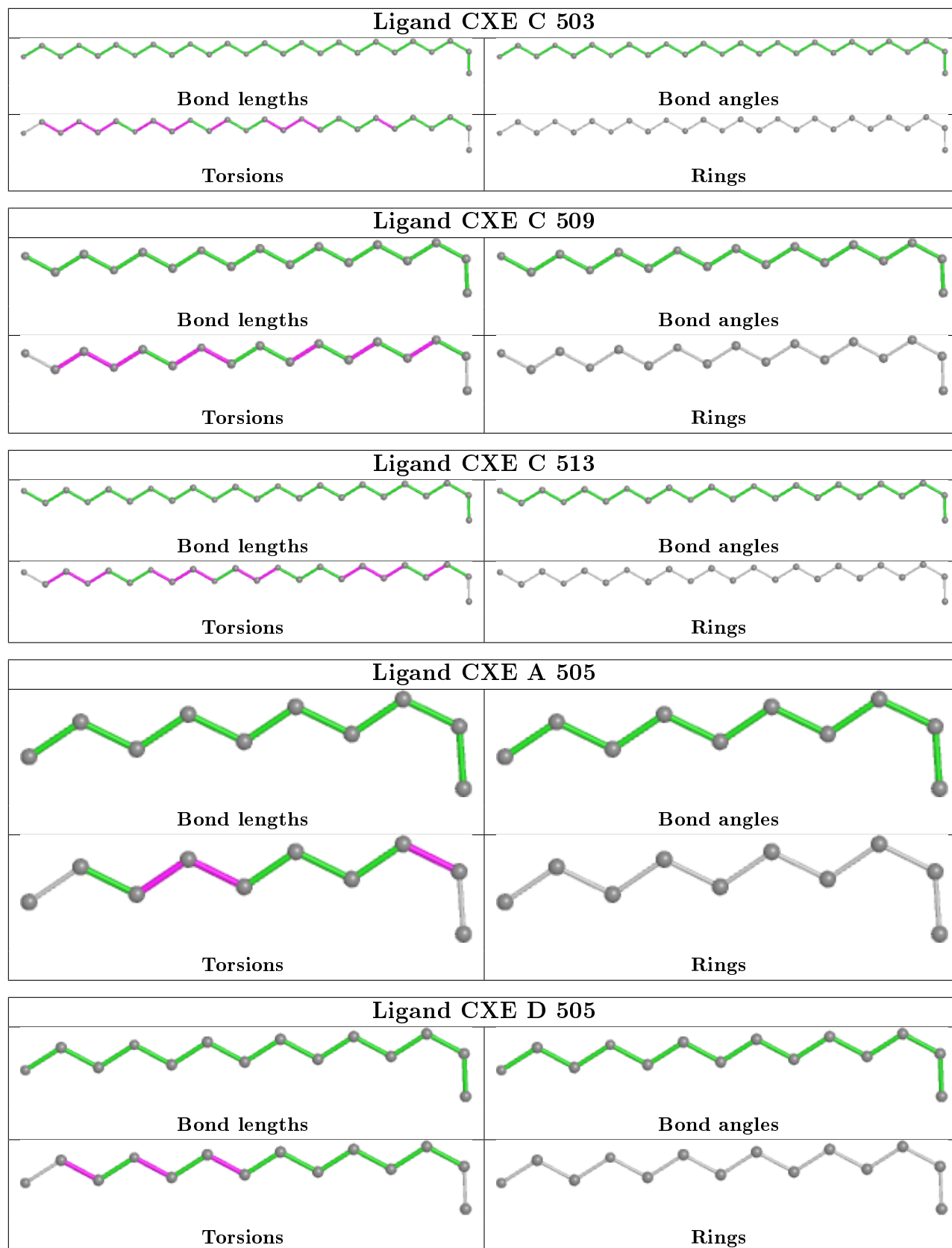


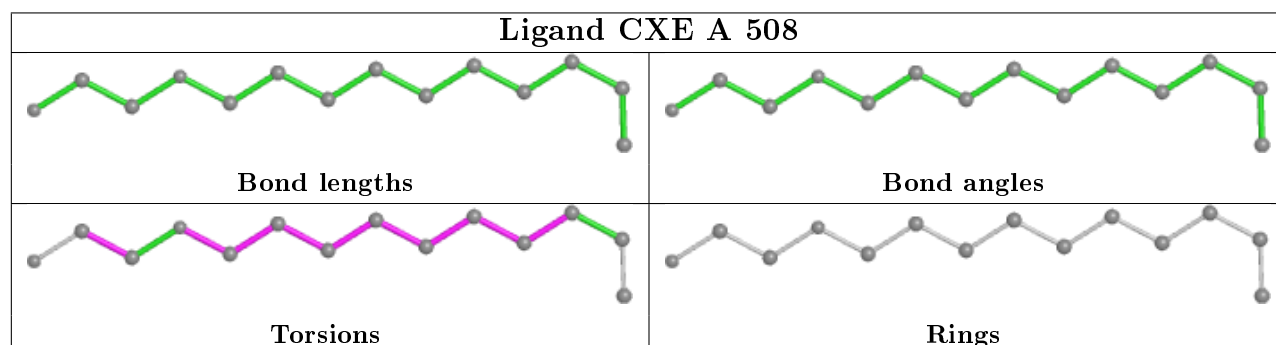
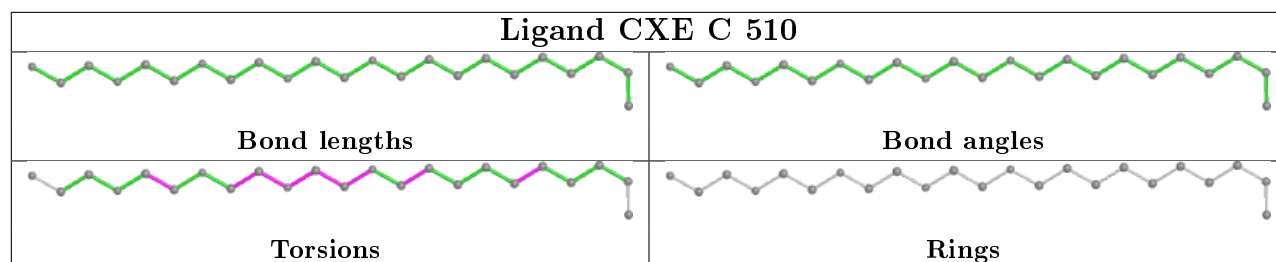
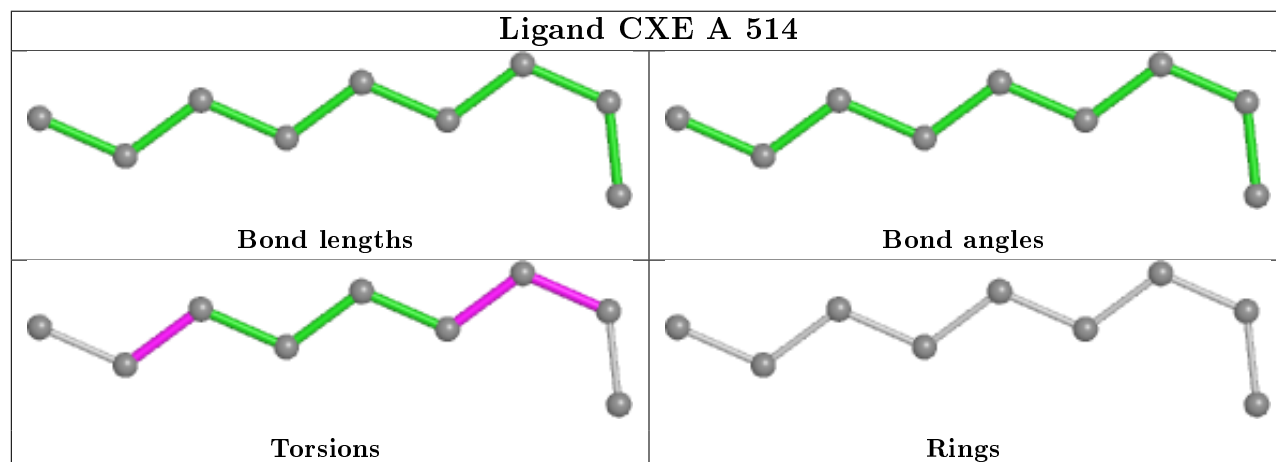
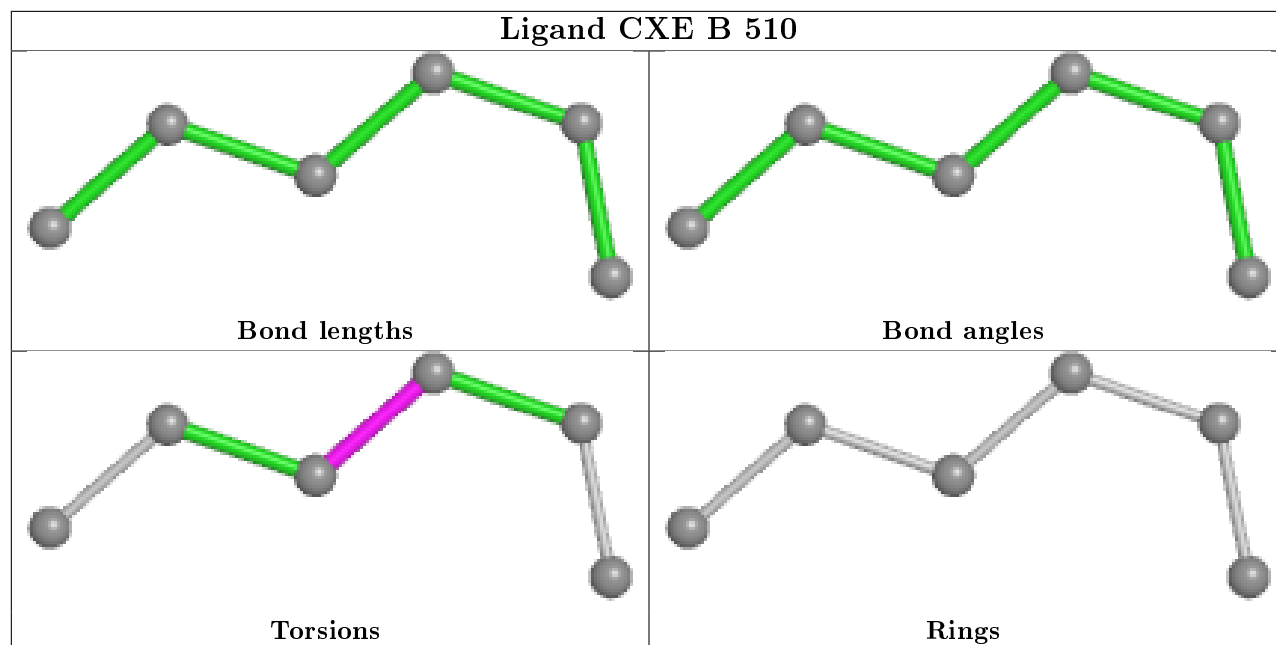


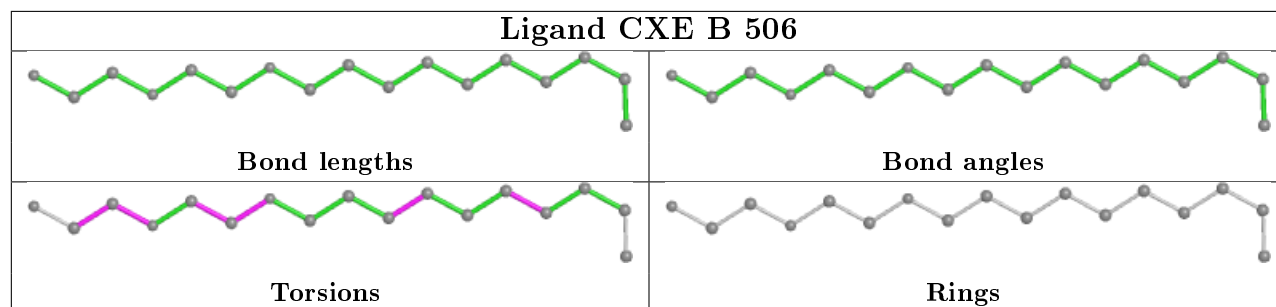
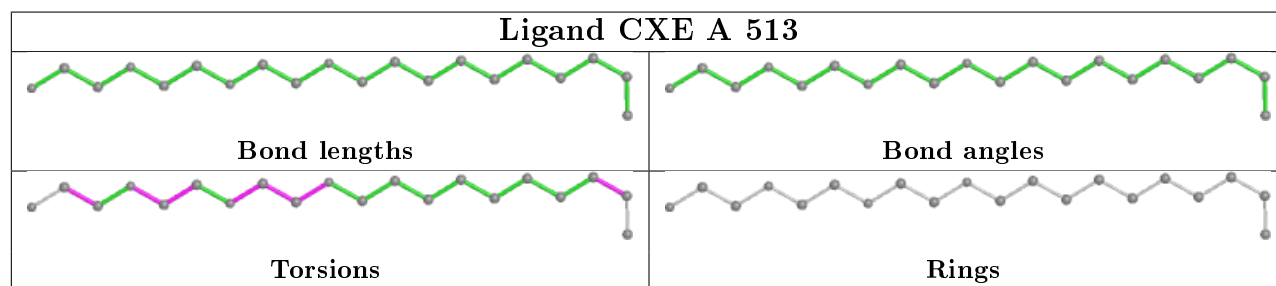
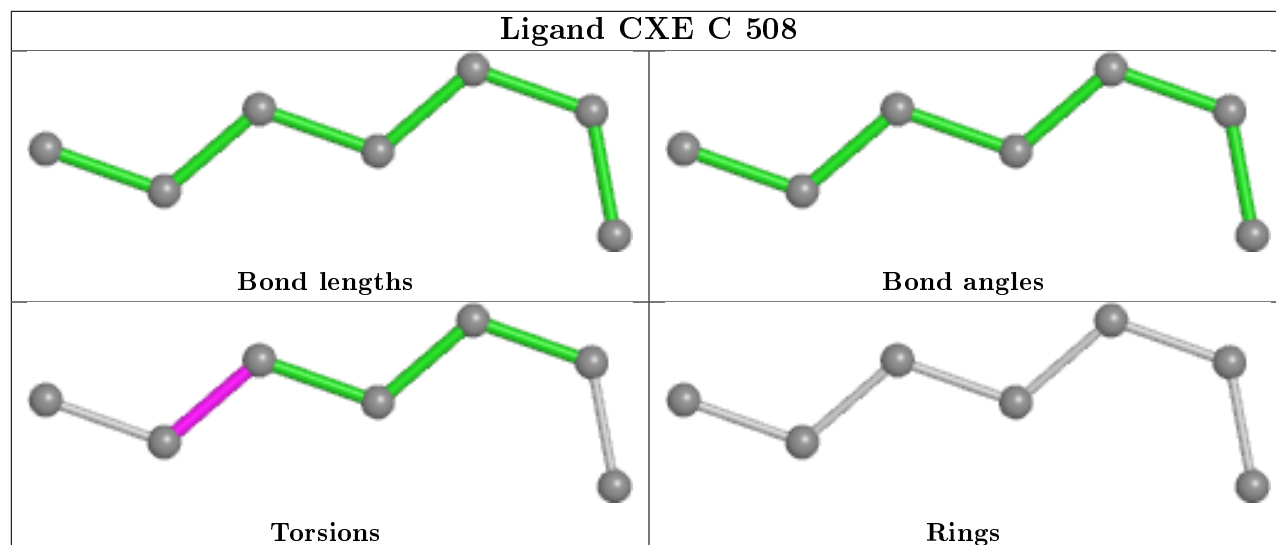


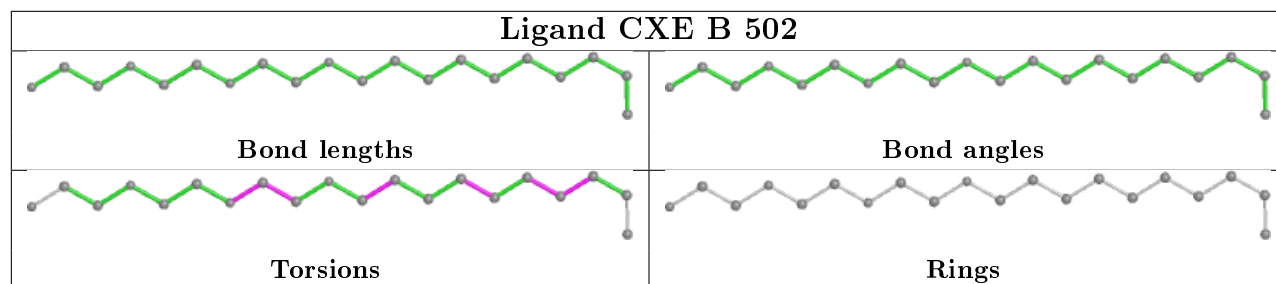
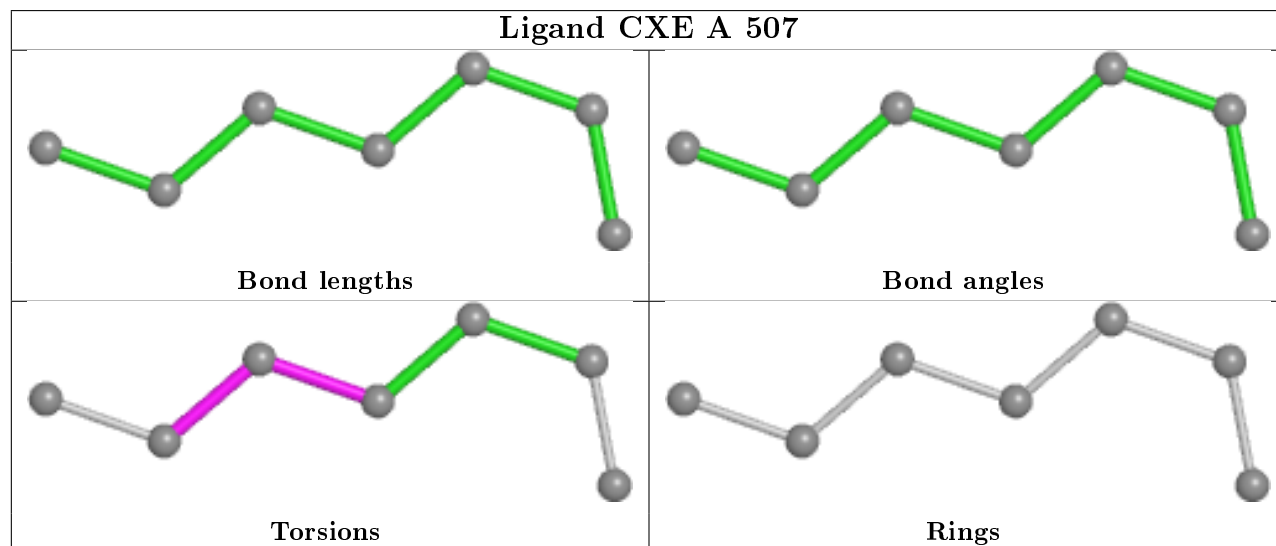
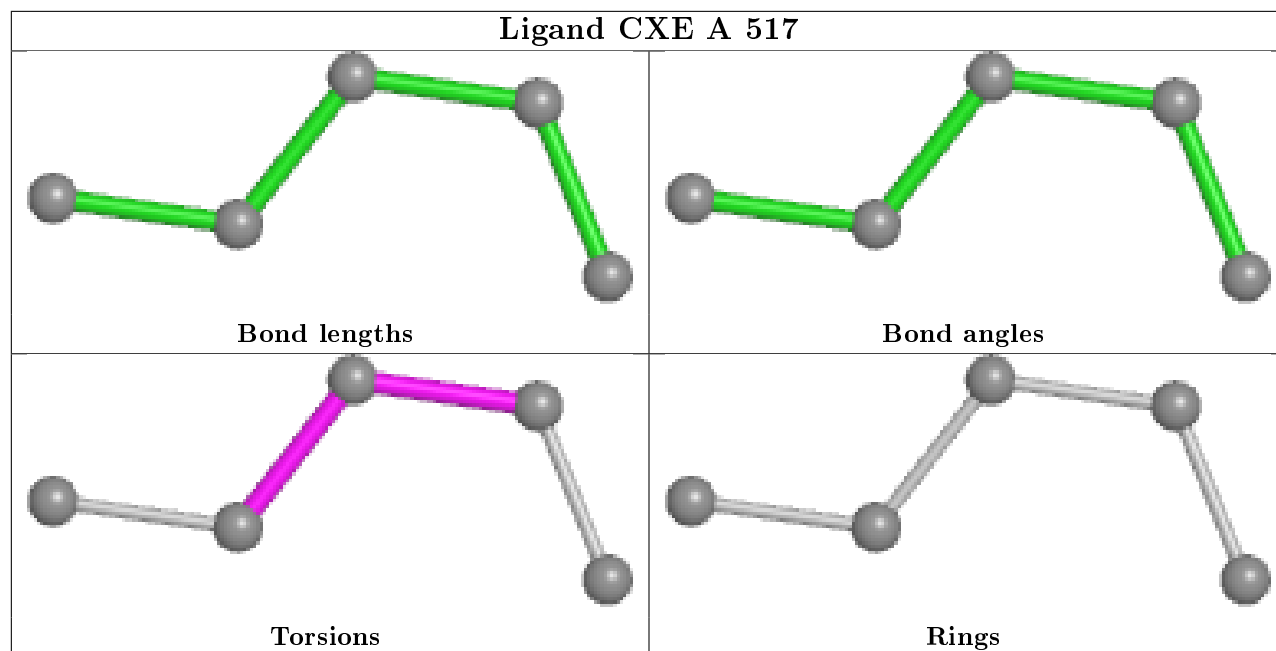


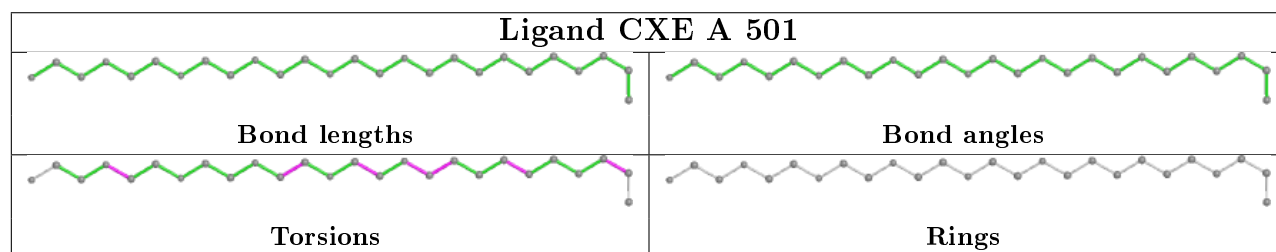
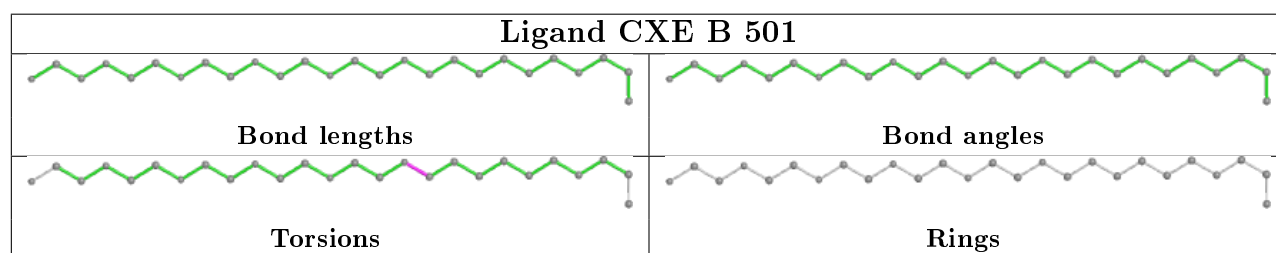
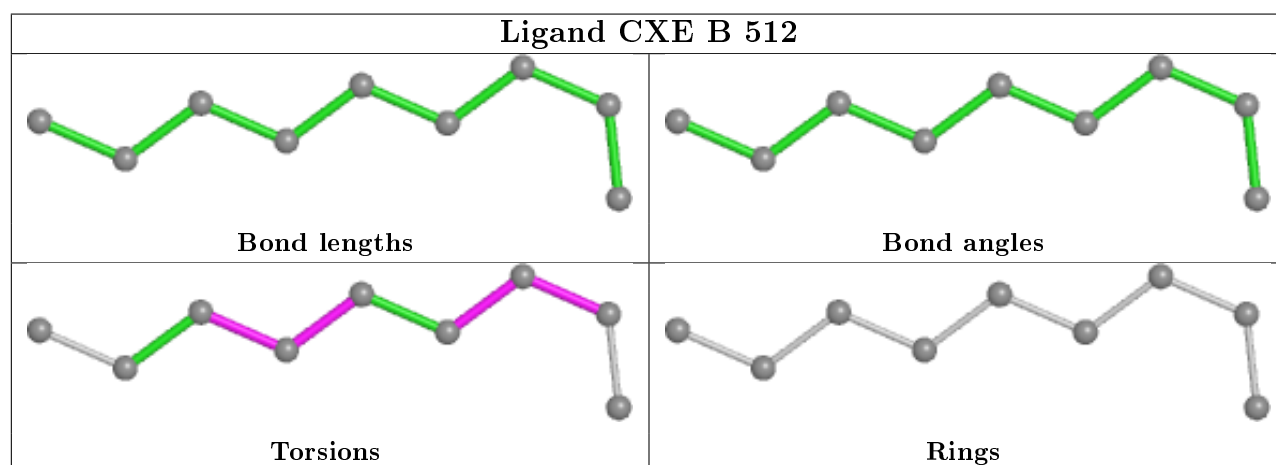
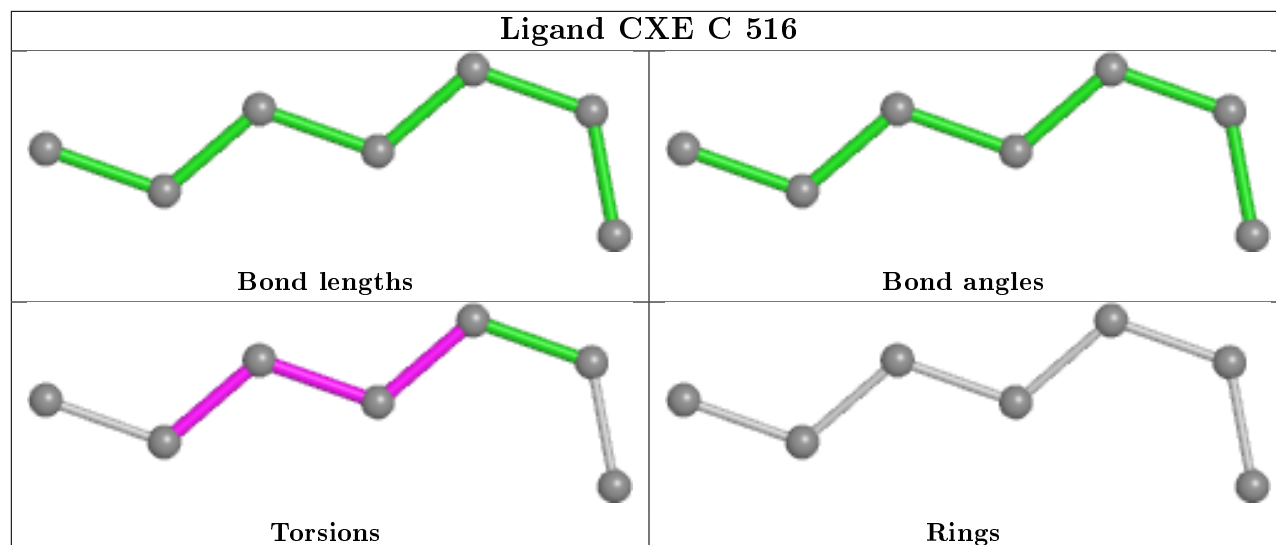


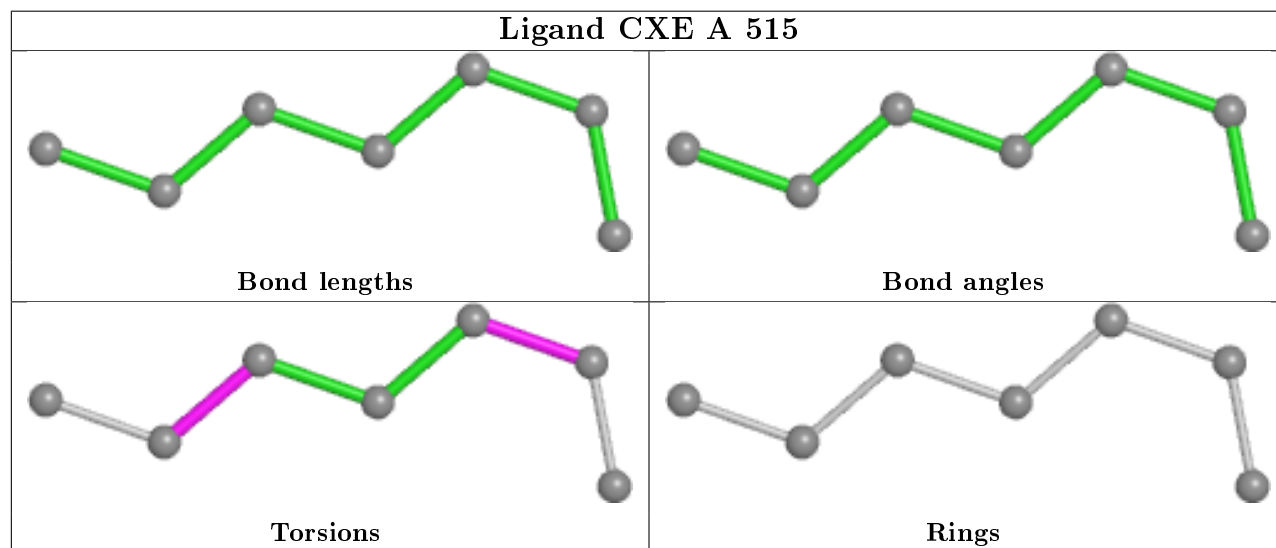
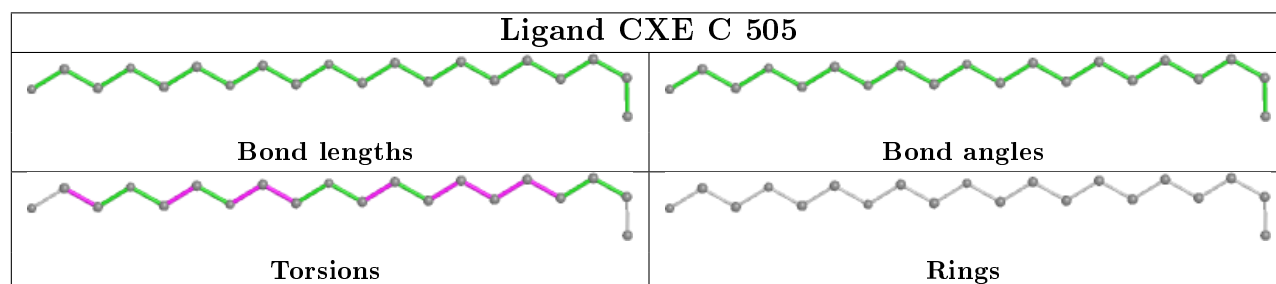
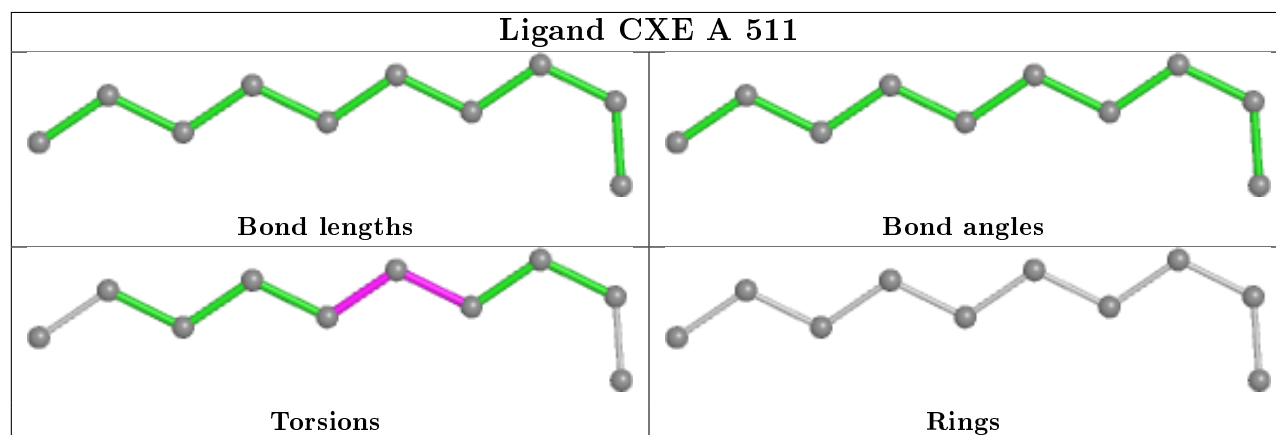
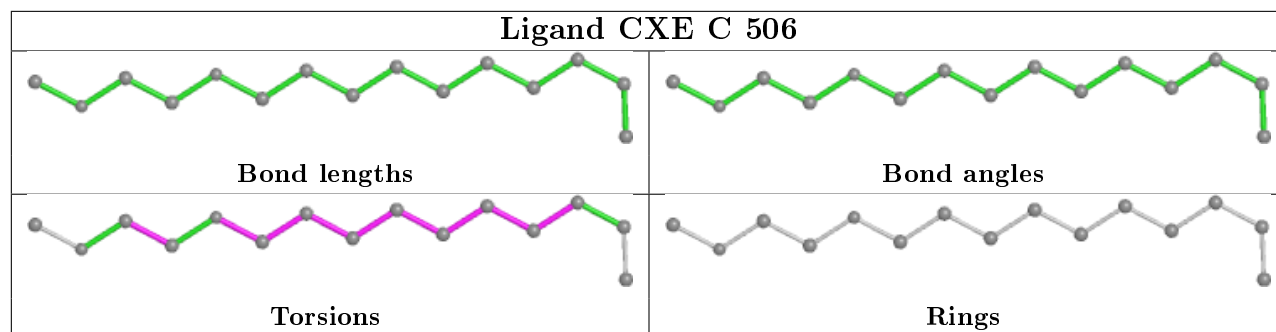


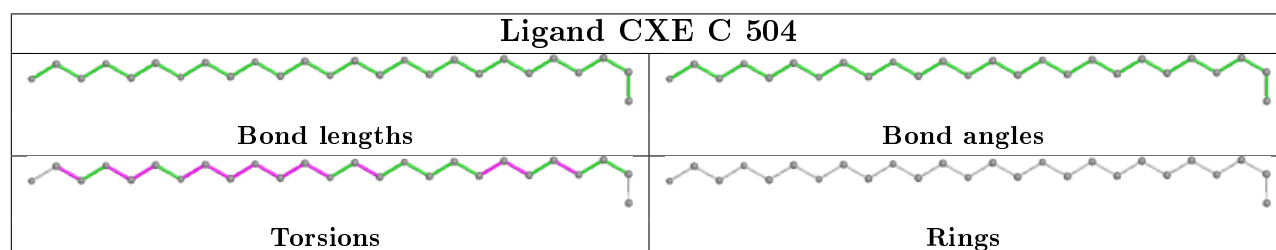
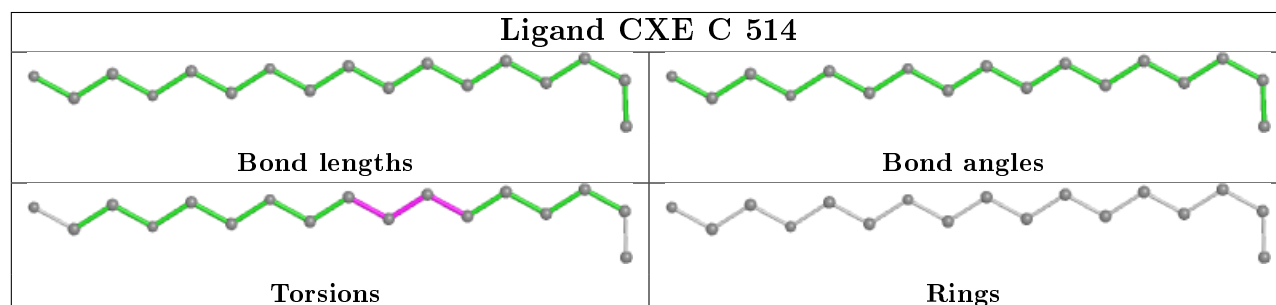
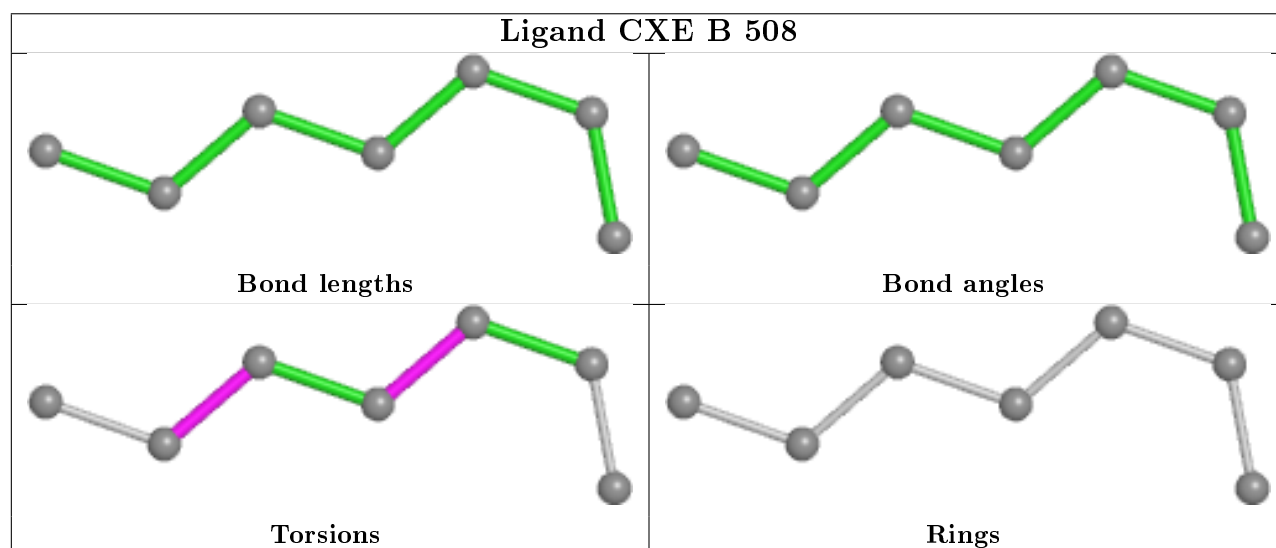
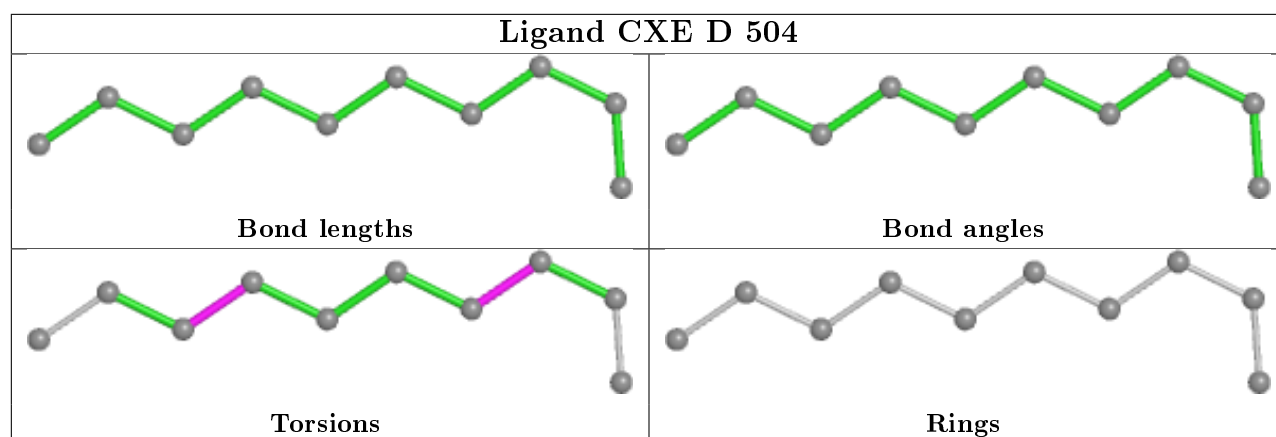


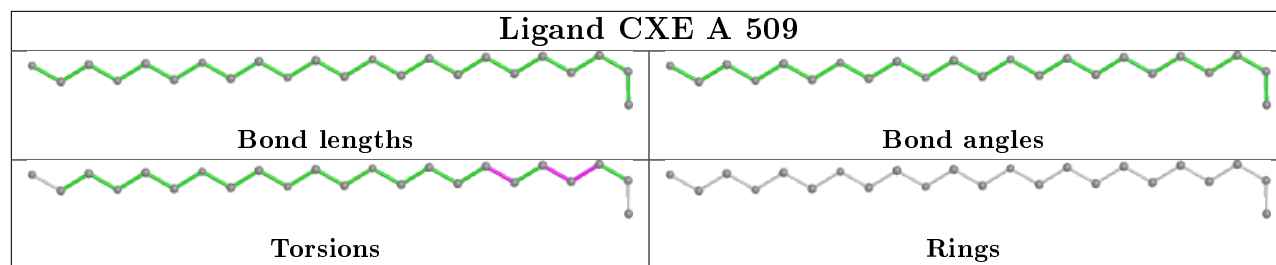












5.7 Other polymers [i](#)

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	453/492 (92%)	0.26	44 (9%) 7 12	19, 37, 89, 146	0
1	B	454/492 (92%)	0.27	28 (6%) 20 28	21, 42, 76, 113	0
1	C	452/492 (91%)	0.40	43 (9%) 8 13	19, 35, 105, 142	0
1	D	452/492 (91%)	0.63	55 (12%) 4 7	33, 53, 97, 129	0
All	All	1811/1968 (92%)	0.39	170 (9%) 8 13	19, 44, 91, 146	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	354	SER	10.9
1	A	456	ALA	8.8
1	D	352	SER	8.0
1	A	454	THR	7.7
1	D	355	ALA	7.3
1	C	353	GLU	7.2
1	D	357	VAL	7.0
1	A	351	TYR	7.0
1	A	347	TYR	6.9
1	A	352	SER	6.7
1	C	350	THR	6.7
1	B	357	VAL	6.4
1	D	454	THR	6.2
1	A	455	SER	6.2
1	C	357	VAL	6.0
1	C	4	LYS	5.9
1	C	267	ALA	5.7
1	C	270	ALA	5.7
1	A	126	MET	5.7
1	A	355	ALA	5.7
1	A	350	THR	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	356	GLN	5.6
1	D	231	ASP	5.6
1	C	355	ALA	5.5
1	C	127	GLY	5.3
1	D	228	THR	5.3
1	D	59	PHE	5.2
1	D	128	ALA	5.0
1	D	129	LYS	5.0
1	D	232	PHE	5.0
1	C	271	GLY	4.9
1	C	276	VAL	4.8
1	D	126	MET	4.8
1	B	273	GLU	4.8
1	D	354	SER	4.8
1	B	352	SER	4.7
1	D	130	GLY	4.7
1	C	358	ILE	4.7
1	C	261	PHE	4.7
1	C	126	MET	4.6
1	C	264	ASN	4.6
1	D	353	GLU	4.5
1	C	275	GLY	4.4
1	C	263	LEU	4.4
1	C	279	PHE	4.4
1	A	273	GLU	4.2
1	D	133	VAL	4.2
1	D	131	GLU	4.0
1	B	354	SER	4.0
1	B	232	PHE	4.0
1	C	283	TRP	3.9
1	A	340	LEU	3.9
1	D	229	LEU	3.9
1	A	357	VAL	3.9
1	B	129	LYS	3.8
1	C	266	VAL	3.8
1	A	271	GLY	3.8
1	B	355	ALA	3.8
1	B	3	GLU	3.7
1	D	124	ARG	3.7
1	B	126	MET	3.6
1	B	127	GLY	3.6
1	D	127	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	123	PHE	3.5
1	A	231	ASP	3.5
1	B	233	SER	3.5
1	B	272	GLY	3.5
1	A	358	ILE	3.4
1	C	351	TYR	3.4
1	A	353	GLU	3.4
1	A	346	ALA	3.4
1	C	125	SER	3.4
1	A	272	GLY	3.4
1	D	138	GLU	3.4
1	D	240	LYS	3.4
1	A	361	ASP	3.3
1	D	135	LEU	3.3
1	C	454	THR	3.3
1	D	122	LEU	3.3
1	C	268	ILE	3.2
1	B	311	ARG	3.2
1	D	340	LEU	3.2
1	D	351	TYR	3.2
1	B	287	MET	3.2
1	A	453	LYS	3.2
1	C	273	GLU	3.1
1	C	370	PRO	3.1
1	C	426	TRP	3.1
1	C	341	PHE	3.1
1	D	116	LEU	3.1
1	A	232	PHE	3.1
1	D	132	ALA	3.1
1	A	419	THR	3.0
1	B	353	GLU	3.0
1	A	127	GLY	3.0
1	A	268	ILE	3.0
1	B	231	ASP	3.0
1	D	113	ILE	3.0
1	A	339	MET	3.0
1	A	261	PHE	3.0
1	C	349	PHE	3.0
1	D	121	SER	2.9
1	D	359	LYS	2.9
1	C	128	ALA	2.9
1	A	356	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	362	LEU	2.9
1	D	137	ILE	2.9
1	A	4	LYS	2.9
1	D	350	THR	2.9
1	B	125	SER	2.9
1	D	311	ARG	2.9
1	A	354	SER	2.8
1	B	4	LYS	2.8
1	A	360	GLY	2.8
1	D	230	ARG	2.8
1	C	272	GLY	2.8
1	D	233	SER	2.7
1	B	351	TYR	2.7
1	B	342	ALA	2.7
1	D	119	ILE	2.7
1	C	3	GLU	2.7
1	B	358	ILE	2.6
1	A	349	PHE	2.6
1	D	453	LYS	2.6
1	A	122	LEU	2.6
1	A	420	LEU	2.6
1	C	421	GLY	2.5
1	B	453	LYS	2.5
1	C	260	MET	2.5
1	D	141	ARG	2.5
1	D	117	PRO	2.4
1	A	274	ASN	2.4
1	A	426	TRP	2.4
1	B	356	GLN	2.4
1	B	128	ALA	2.4
1	C	262	PHE	2.4
1	D	215	TYR	2.4
1	C	287	MET	2.4
1	A	262	PHE	2.3
1	A	125	SER	2.3
1	B	229	LEU	2.3
1	B	7	LYS	2.3
1	C	123	PHE	2.3
1	C	356	GLN	2.3
1	D	114	THR	2.3
1	A	365	ALA	2.3
1	D	125	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	269	THR	2.2
1	A	348	LEU	2.2
1	D	120	ASP	2.2
1	C	347	TYR	2.2
1	C	122	LEU	2.2
1	C	362	LEU	2.2
1	A	336	ALA	2.2
1	A	129	LYS	2.2
1	A	342	ALA	2.2
1	D	358	ILE	2.2
1	D	115	MET	2.2
1	D	343	PRO	2.2
1	D	5	THR	2.1
1	B	274	ASN	2.1
1	D	136	ALA	2.1
1	D	287	MET	2.1
1	D	341	PHE	2.1
1	C	129	LYS	2.0
1	D	94	ASP	2.0
1	A	366	LEU	2.0
1	B	362	LEU	2.0
1	D	134	GLU	2.0
1	D	238	ILE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

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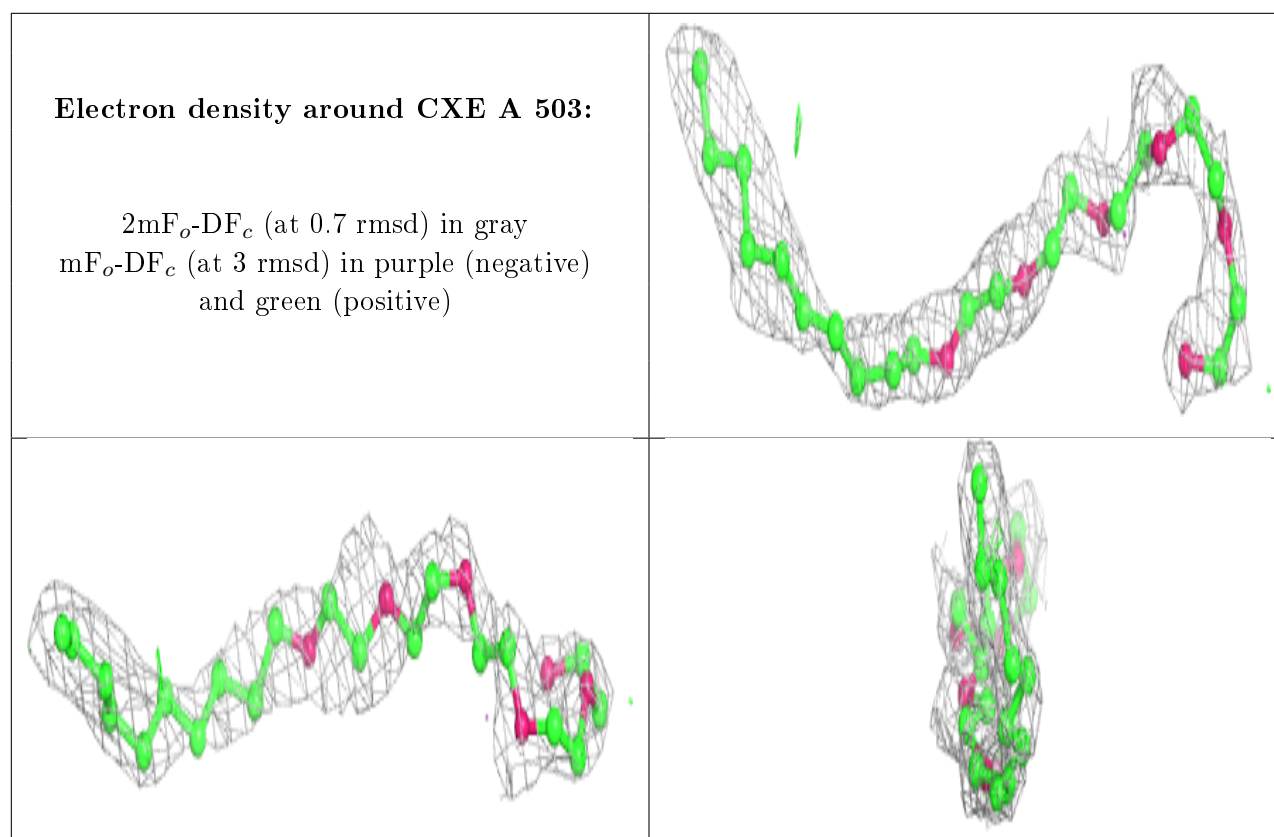
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CXE	A	503	26/26	0.63	0.35	65,77,83,85	0
2	CXE	A	509	23/26	0.63	0.39	56,83,102,104	0
2	CXE	C	514	17/26	0.66	0.34	50,70,93,93	0
2	CXE	B	511	6/26	0.71	1.05	34,38,39,42	6
2	CXE	A	508	14/26	0.71	0.29	63,78,100,100	0
2	CXE	A	513	20/26	0.73	0.26	42,74,102,106	0
2	CXE	C	505	20/26	0.73	0.27	46,62,82,83	0
2	CXE	C	504	26/26	0.74	0.38	50,72,102,105	0
2	CXE	C	503	26/26	0.75	0.24	47,57,74,78	0
2	CXE	D	505	14/26	0.76	0.24	49,66,77,78	0
2	CXE	B	512	9/26	0.78	0.23	44,53,62,65	0
2	CXE	D	506	11/26	0.78	0.23	64,68,87,91	0
2	CXE	C	501	26/26	0.78	0.28	26,43,88,95	0
2	CXE	B	505	10/26	0.78	0.21	46,60,72,77	0
2	CXE	C	502	26/26	0.78	0.30	40,76,83,87	0
2	CXE	C	513	23/26	0.79	0.25	57,67,81,85	0
2	CXE	D	504	10/26	0.80	0.22	55,59,73,74	0
2	CXE	B	504	11/26	0.80	0.24	36,74,78,81	0
2	CXE	A	511	10/26	0.80	0.23	58,66,74,74	0
2	CXE	A	507	7/26	0.80	0.17	42,52,59,62	0
2	CXE	B	502	20/26	0.81	0.24	36,50,62,65	0
2	CXE	C	509	17/26	0.81	0.20	54,76,85,95	0
2	CXE	B	506	17/26	0.81	0.22	56,70,84,84	0
2	CXE	A	510	10/26	0.81	0.35	36,63,68,69	0
2	CXE	C	510	23/26	0.83	0.24	49,73,80,88	0
2	CXE	A	501	26/26	0.83	0.18	35,49,60,64	0
2	CXE	B	507	9/26	0.83	0.25	36,61,73,84	0
2	CXE	C	508	7/26	0.83	0.28	52,59,64,66	0
2	CXE	C	512	16/26	0.83	0.25	38,57,82,89	0
2	CXE	D	508	5/26	0.83	0.20	56,57,57,58	0
2	CXE	A	516	7/26	0.83	0.22	52,57,70,73	0
2	CXE	D	507	11/26	0.83	0.23	48,58,67,70	0
2	CXE	A	514	9/26	0.83	0.21	55,62,69,73	0
2	CXE	C	506	15/26	0.84	0.21	37,47,71,75	0
2	CXE	B	503	17/26	0.85	0.21	46,53,66,68	3
2	CXE	B	508	7/26	0.85	0.22	44,52,67,68	0
2	CXE	C	507	10/26	0.85	0.28	60,68,79,80	0
2	CXE	C	511	10/26	0.86	0.23	48,56,65,67	0
2	CXE	A	515	7/26	0.86	0.22	38,53,65,65	0
2	CXE	C	516	7/26	0.86	0.29	51,65,67,68	0
2	CXE	C	515	4/26	0.86	0.15	48,50,54,66	0

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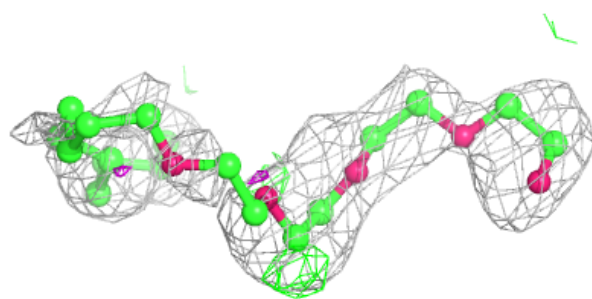
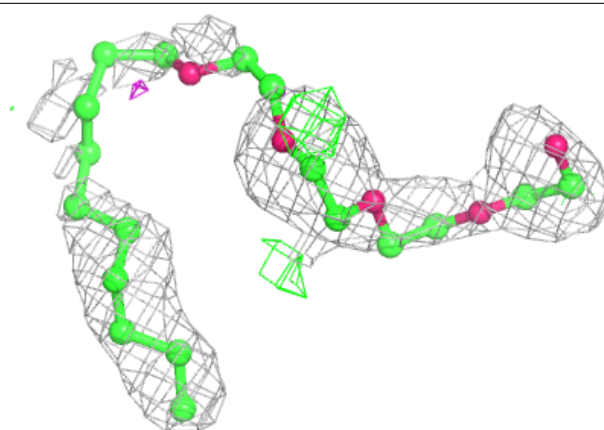
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CXE	B	509	6/26	0.87	1.03	32,36,42,45	6
2	CXE	A	506	20/26	0.87	0.22	24,39,57,58	0
2	CXE	A	502	26/26	0.87	0.25	29,48,74,81	0
2	CXE	A	517	5/26	0.87	0.22	56,60,63,68	0
2	CXE	A	505	10/26	0.87	0.83	38,42,47,63	10
2	CXE	B	510	6/26	0.88	0.14	62,69,71,72	0
2	CXE	A	504	20/26	0.88	0.17	43,61,77,81	0
2	CXE	A	512	6/26	0.88	0.23	34,49,53,65	0
2	CXE	B	501	26/26	0.88	0.19	35,50,77,86	0
2	CXE	D	502	20/26	0.90	0.19	38,48,56,58	10
2	CXE	D	501	11/26	0.91	0.15	41,46,65,65	0
2	CXE	D	503	14/26	0.93	0.17	53,61,65,76	0
3	CL	A	518	1/1	0.97	0.08	29,29,29,29	0
3	CL	A	519	1/1	0.98	0.13	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.



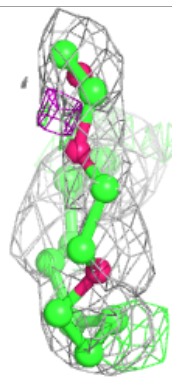
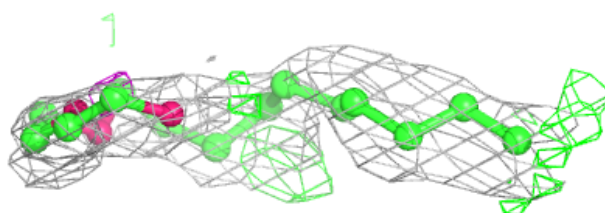
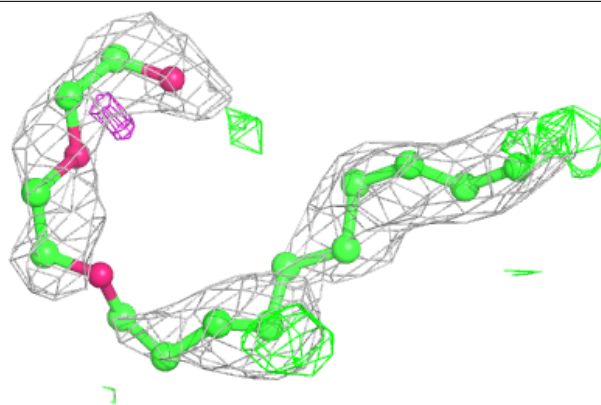
Electron density around CXE A 509:

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

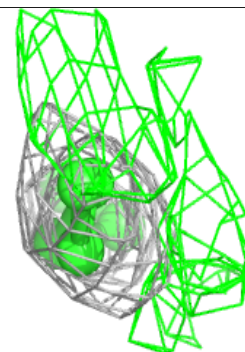
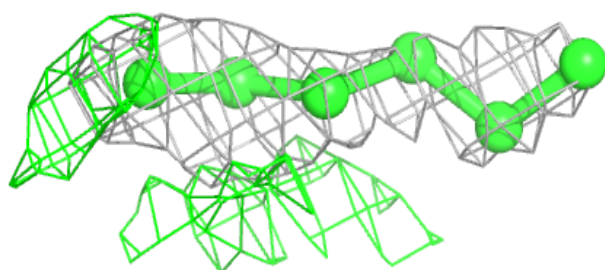
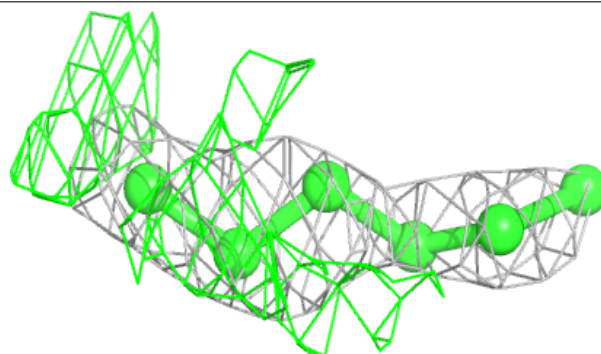


Electron density around CXE C 514:

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

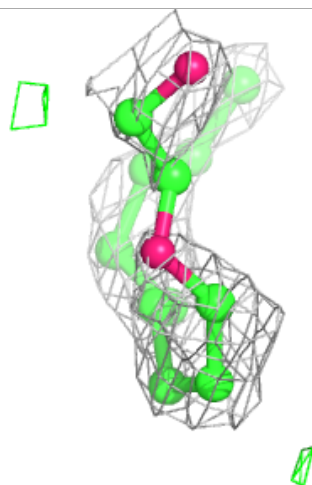
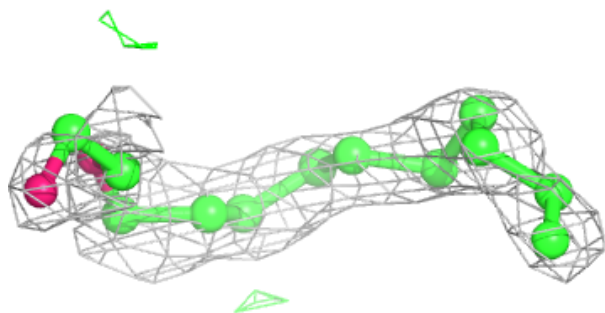
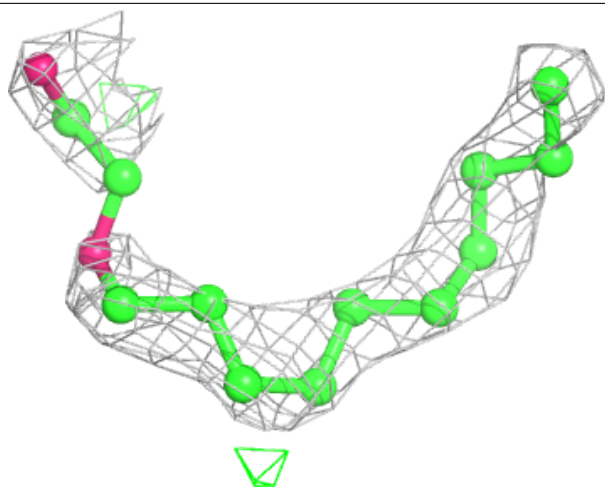
**Electron density around CXE B 511:**

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



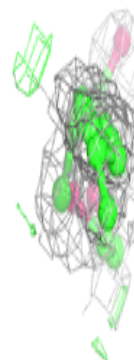
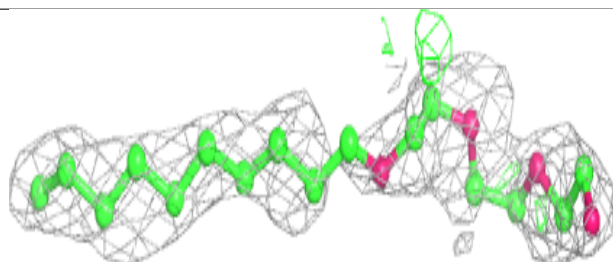
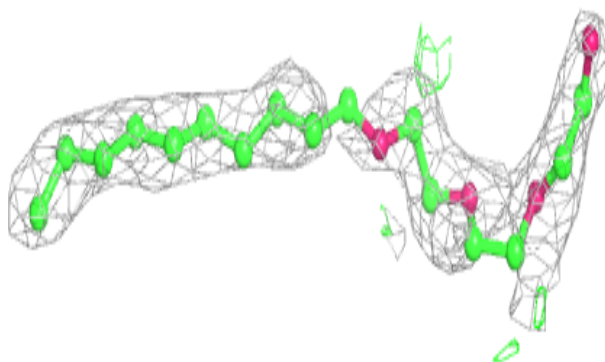
Electron density around CXE A 508:

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

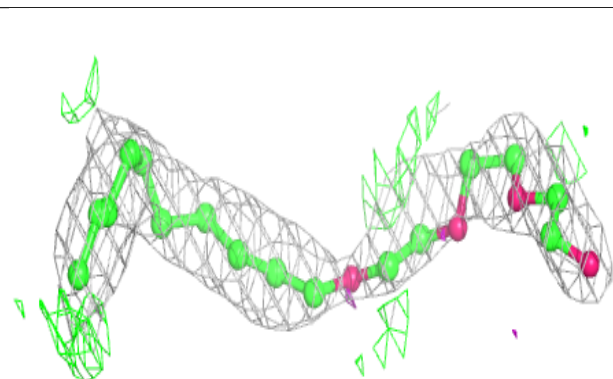
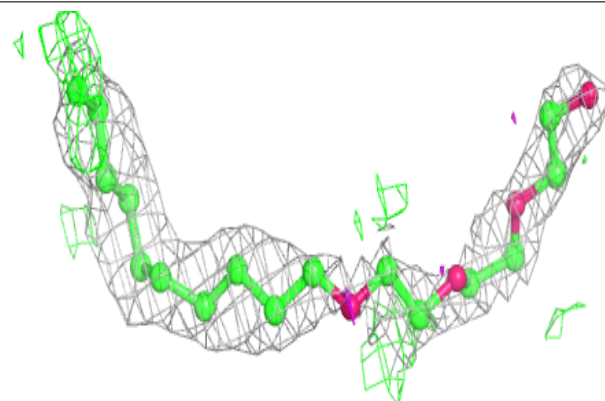


Electron density around CXE A 513:

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

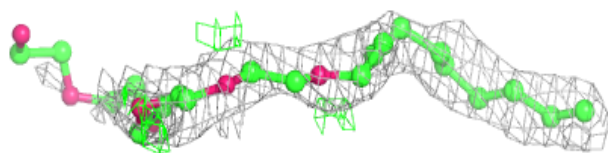
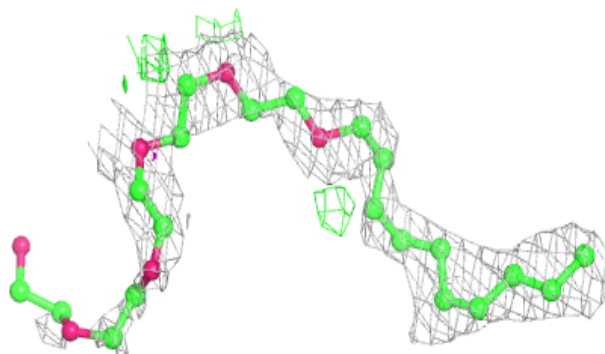
**Electron density around CXE C 505:**

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

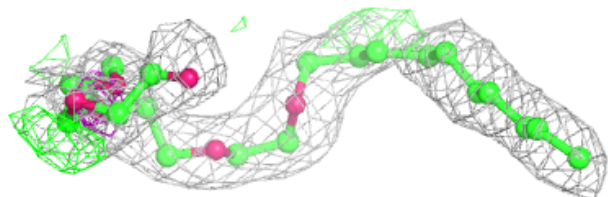
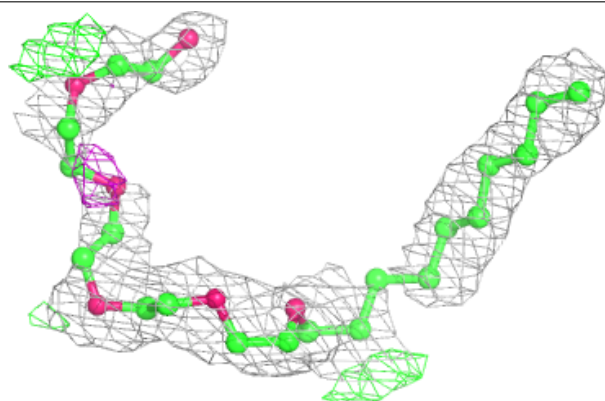


Electron density around CXE C 504:

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

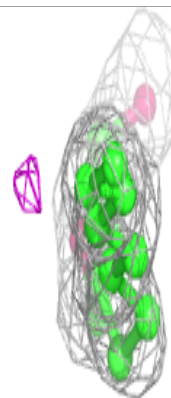
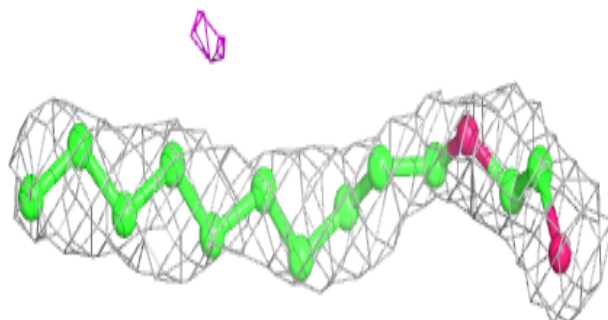
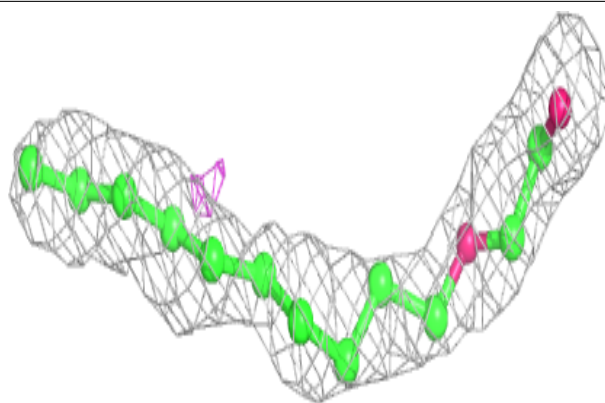
**Electron density around CXE C 503:**

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

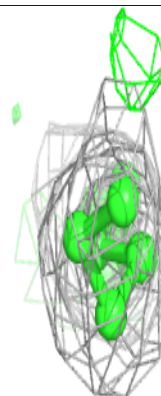
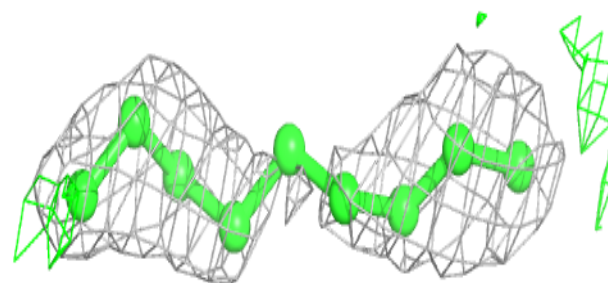
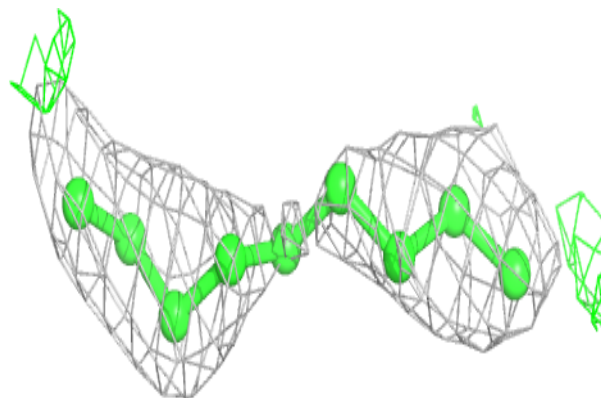


Electron density around CXE D 505:

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

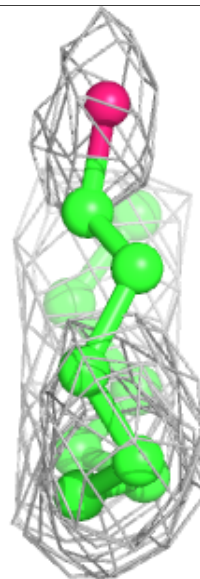
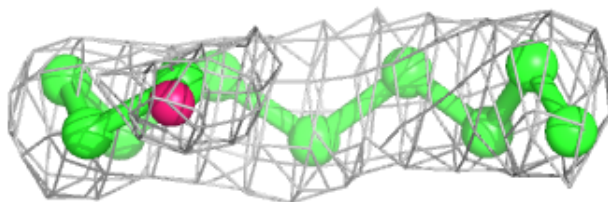
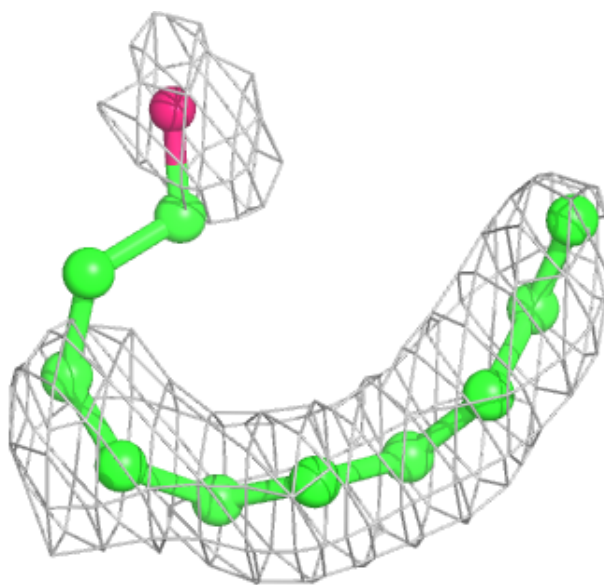
**Electron density around CXE B 512:**

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



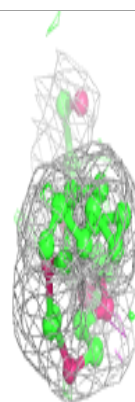
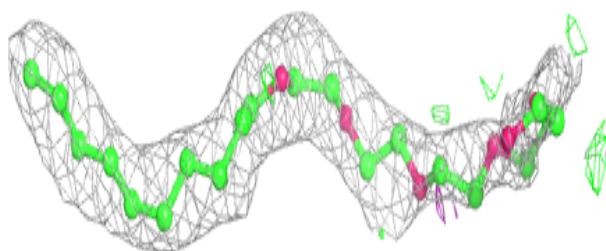
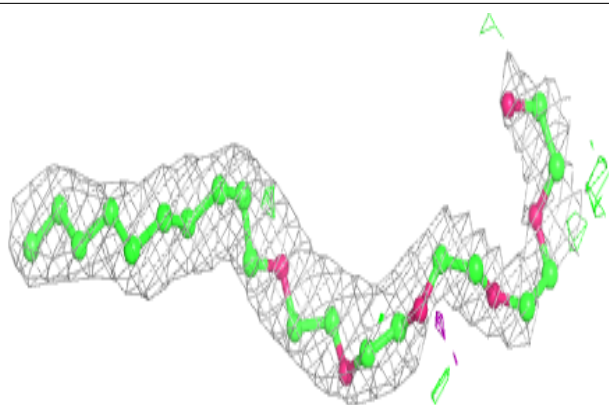
Electron density around CXE D 506:

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

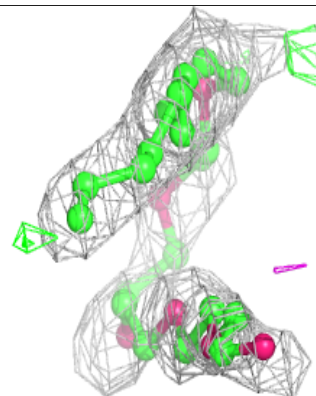
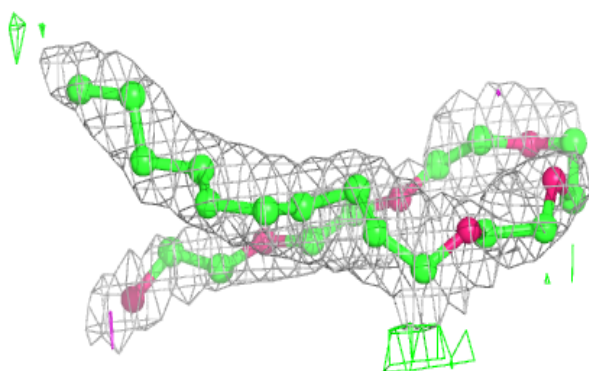
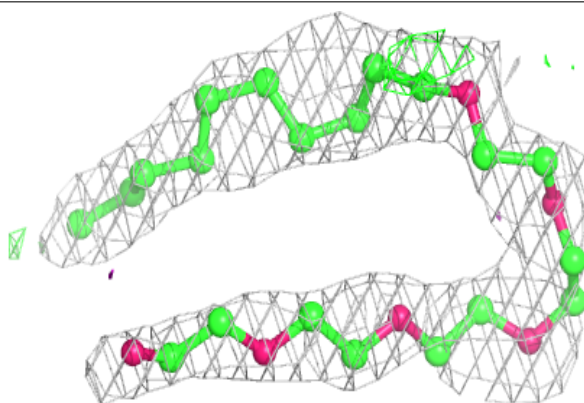


Electron density around CXE C 501:

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

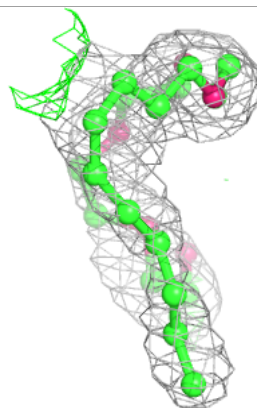
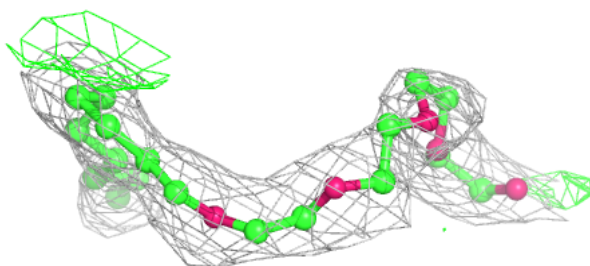
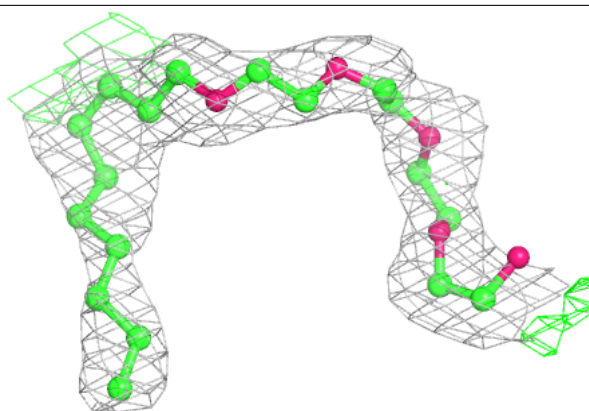
**Electron density around CXE C 502:**

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

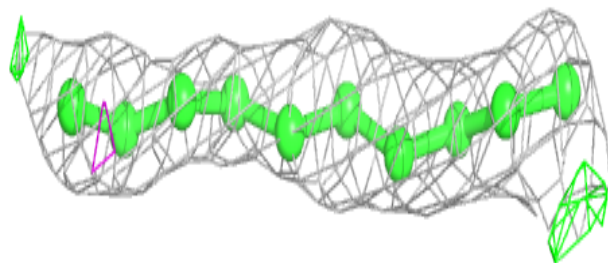
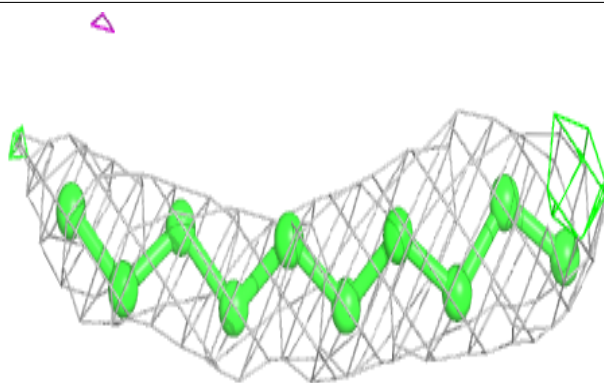


Electron density around CXE C 513:

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

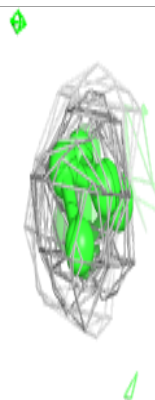
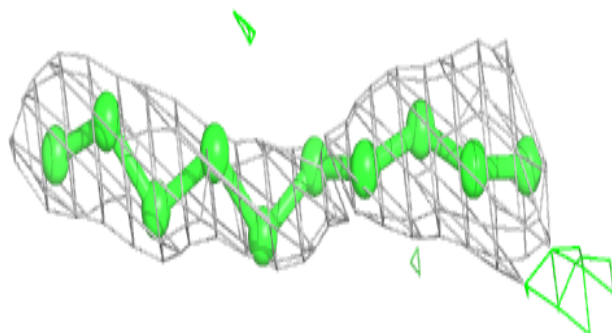
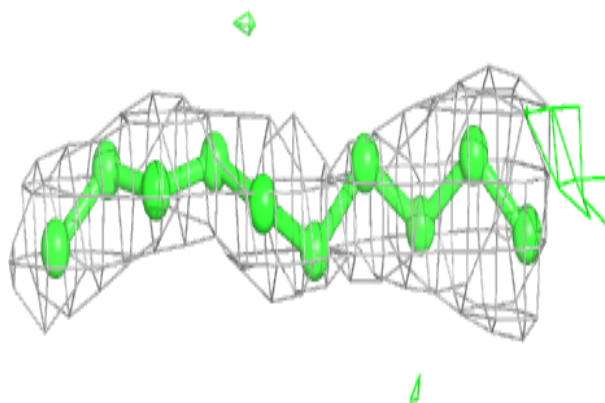
**Electron density around CXE D 504:**

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

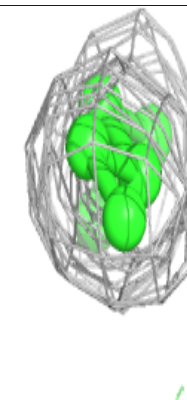
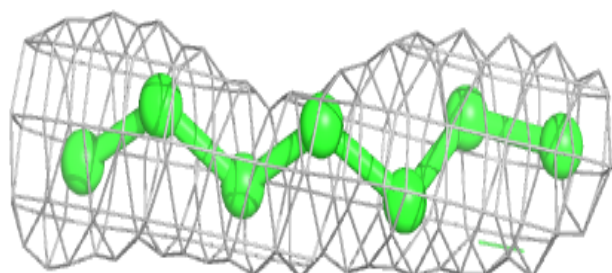
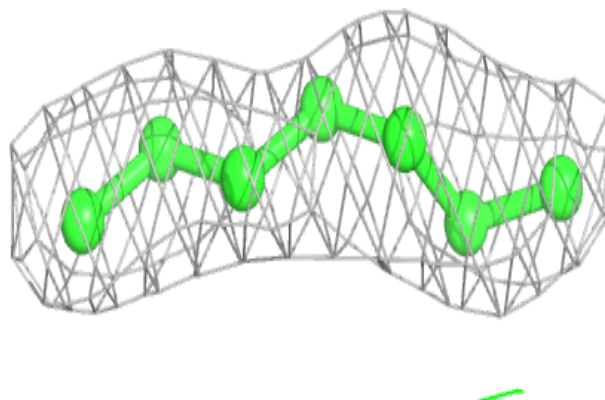


Electron density around CXE A 511:

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

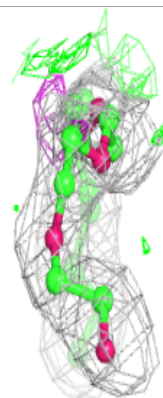
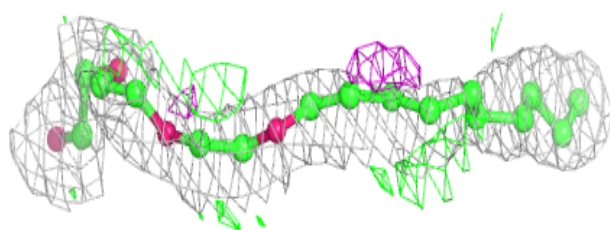
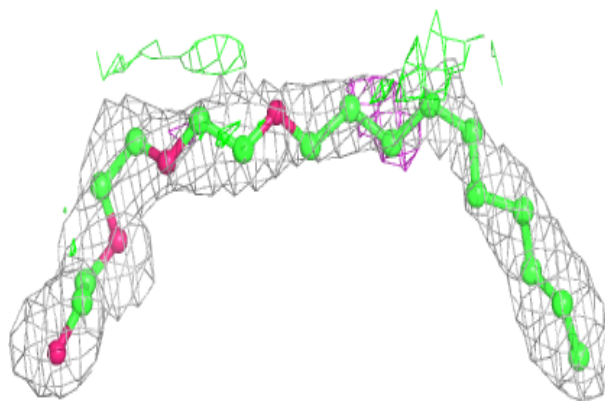
**Electron density around CXE A 507:**

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

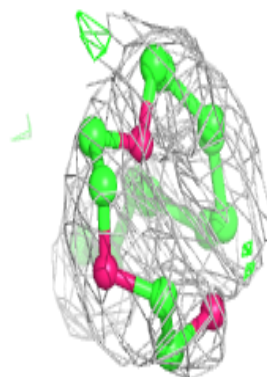
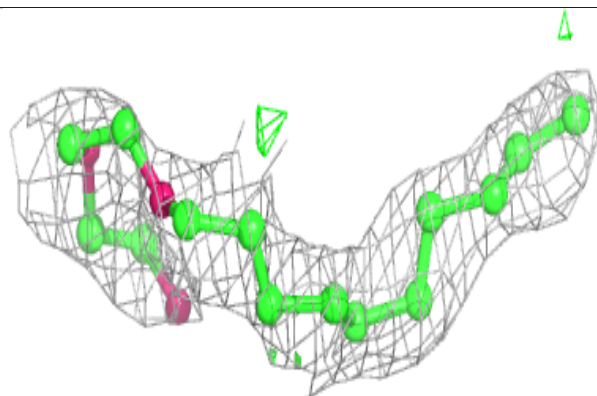
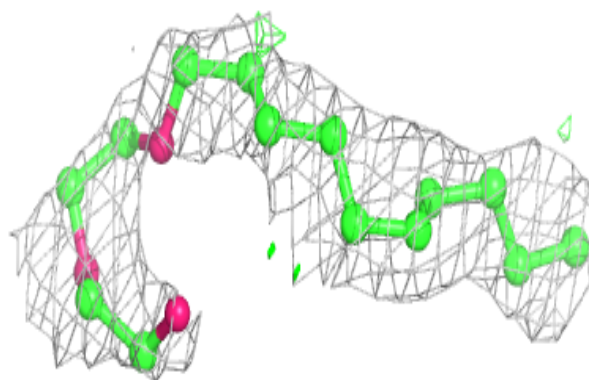


Electron density around CXE B 502:

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

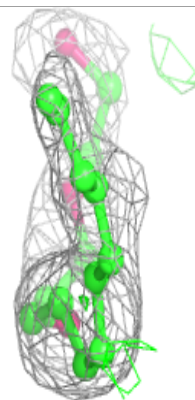
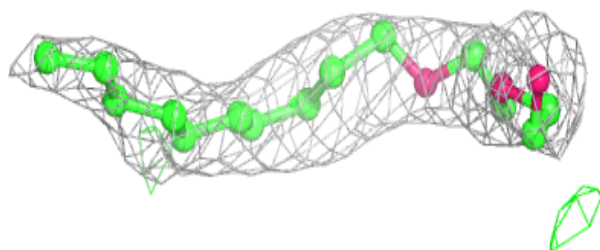
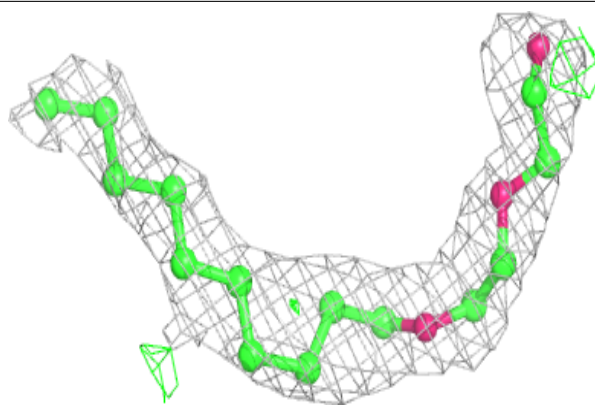
**Electron density around CXE C 509:**

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

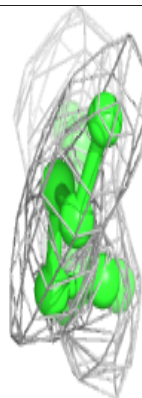
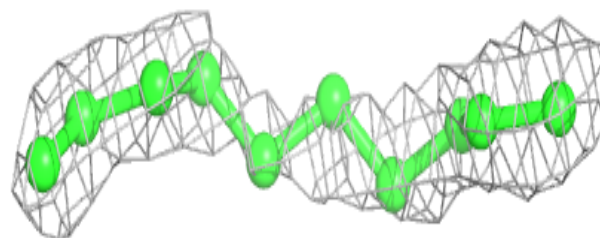
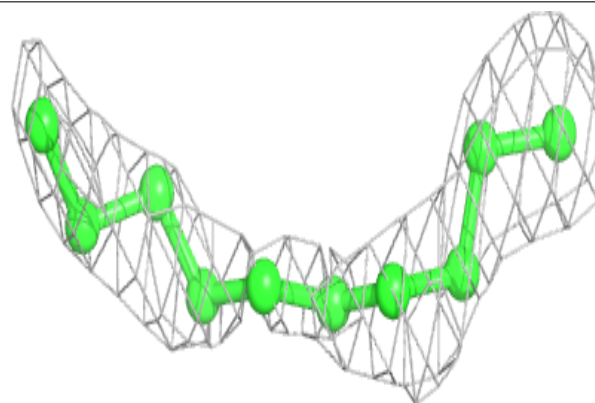


Electron density around CXE B 506:

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

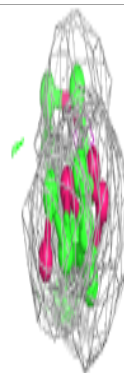
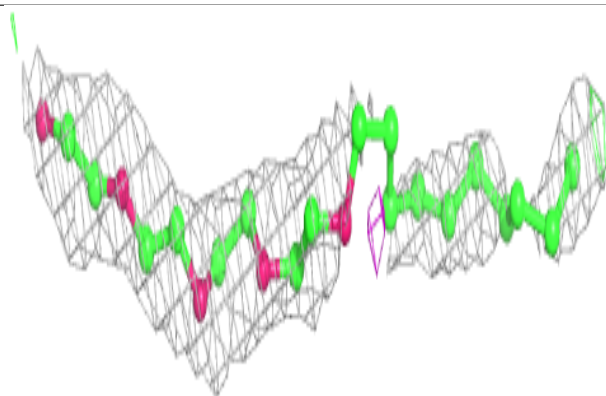
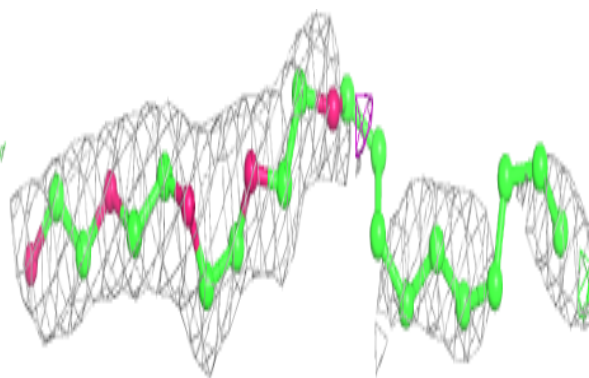
**Electron density around CXE A 510:**

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

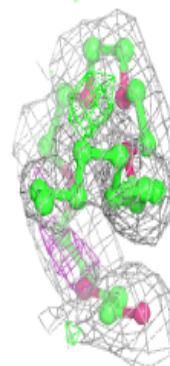
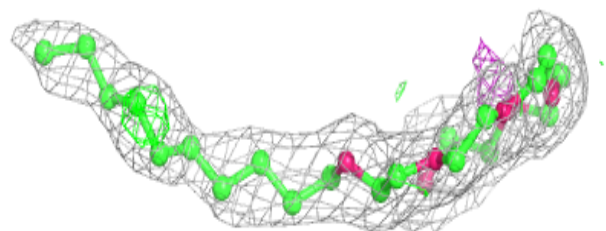
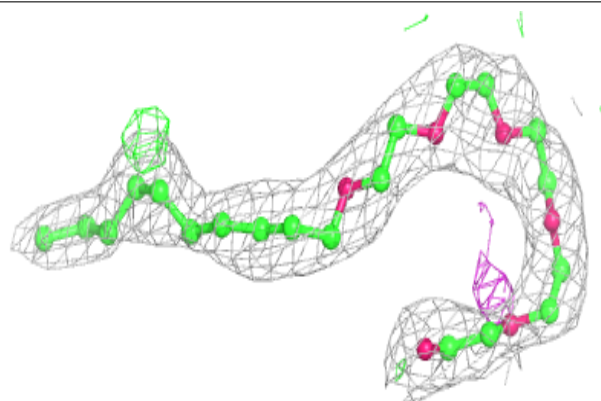


Electron density around CXE C 510:

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

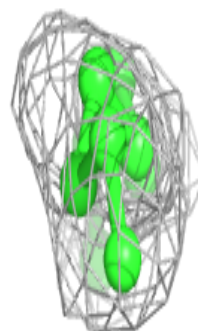
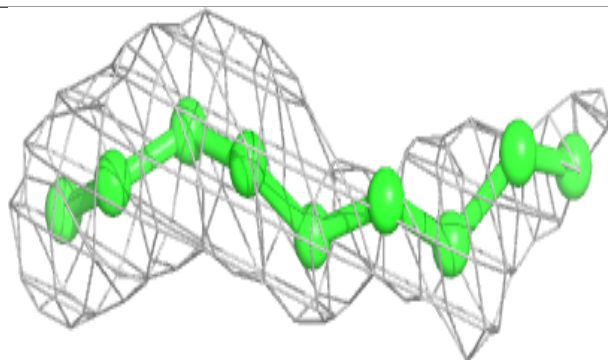
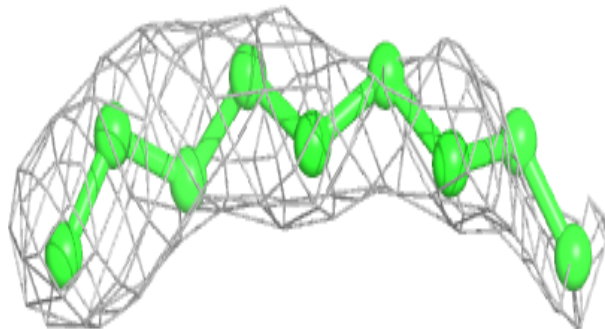
**Electron density around CXE A 501:**

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

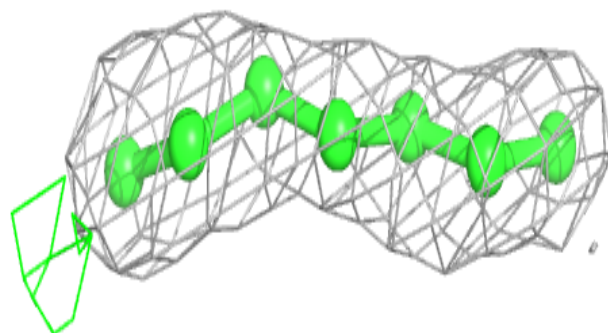
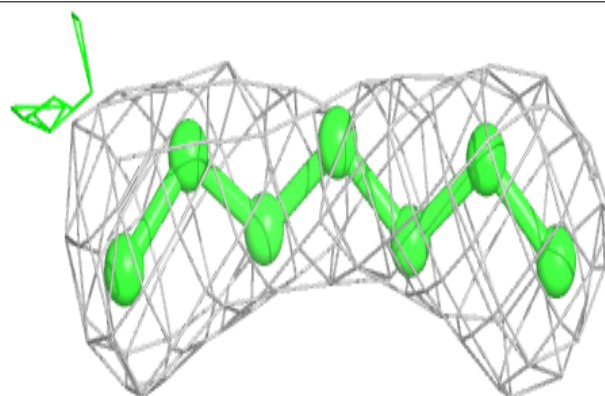


Electron density around CXE B 507:

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

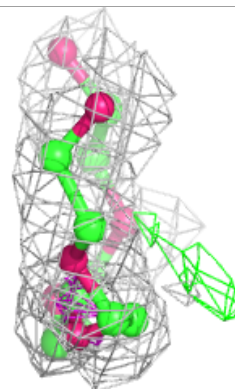
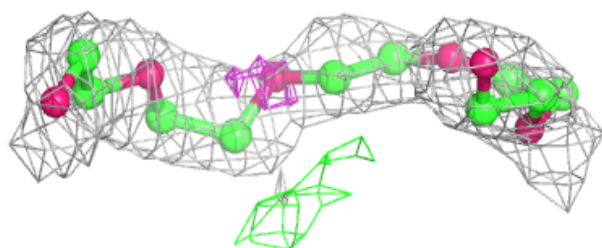
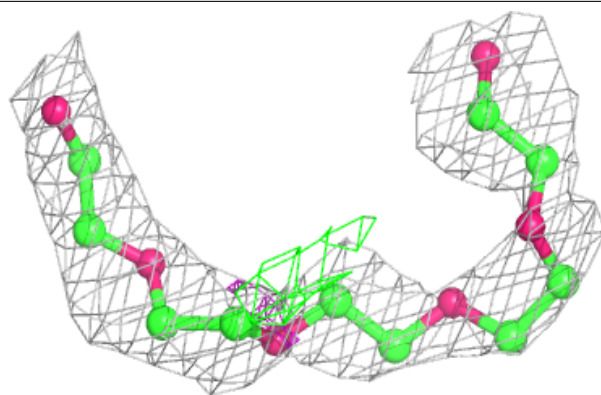
**Electron density around CXE C 508:**

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



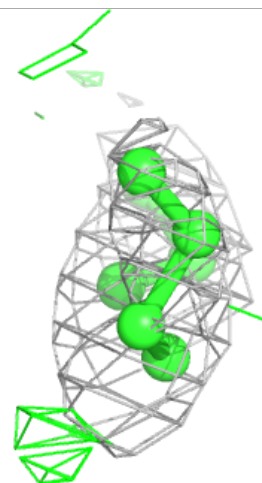
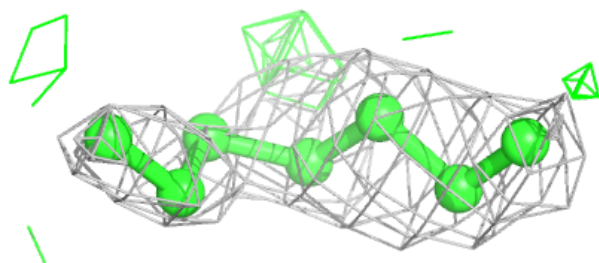
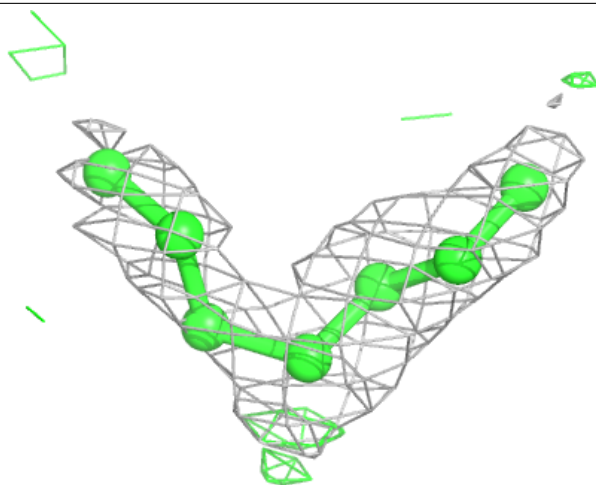
Electron density around CXE C 512:

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



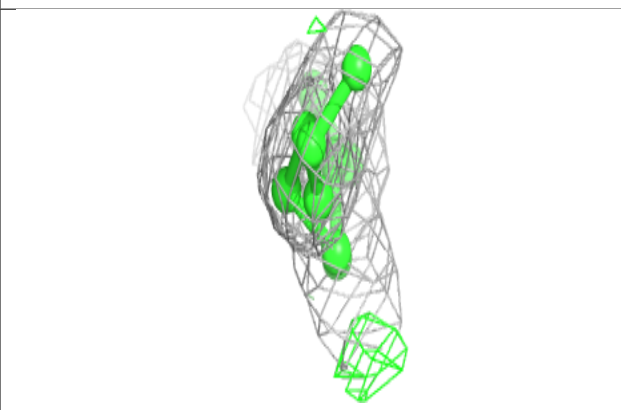
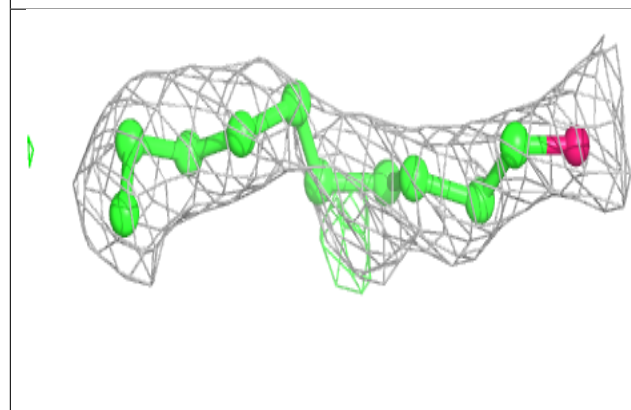
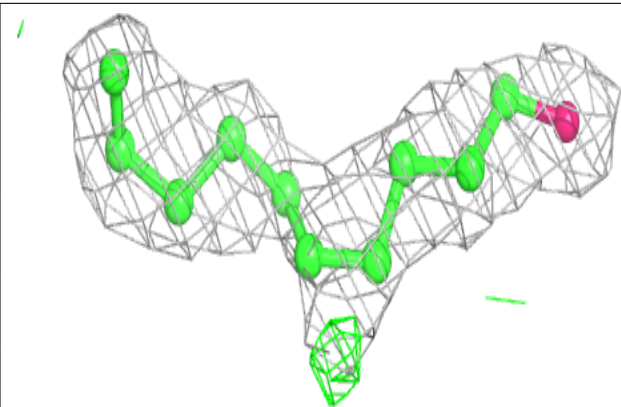
Electron density around CXE A 516:

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

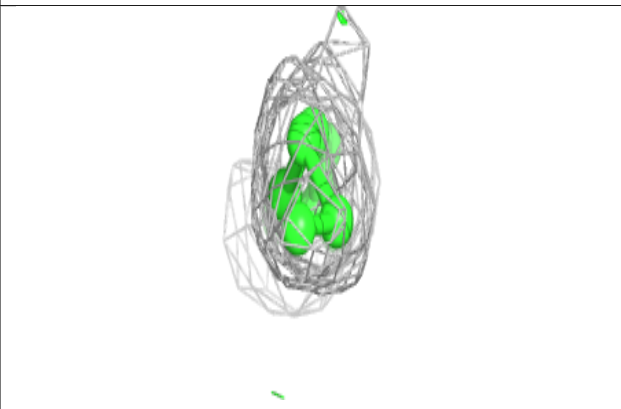
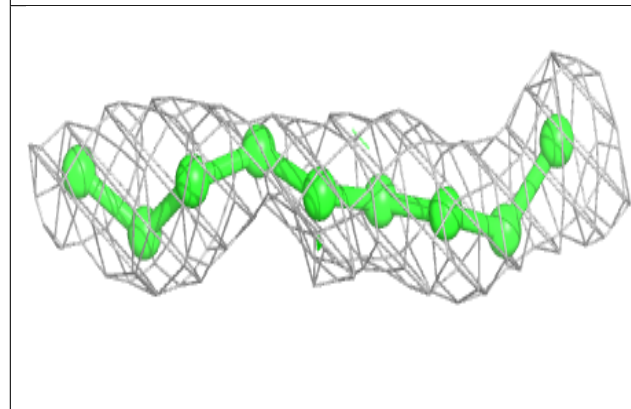
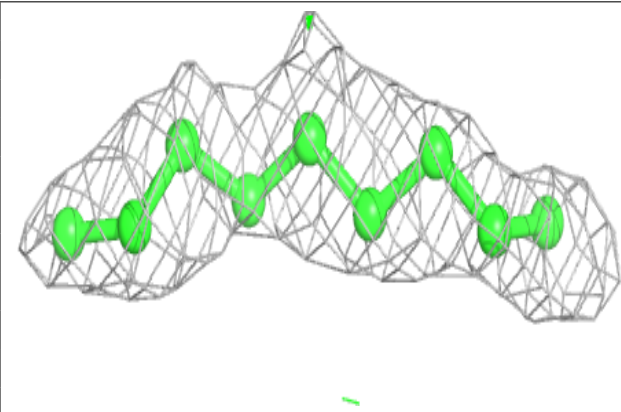


Electron density around CXE D 507:

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

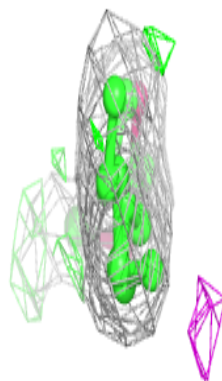
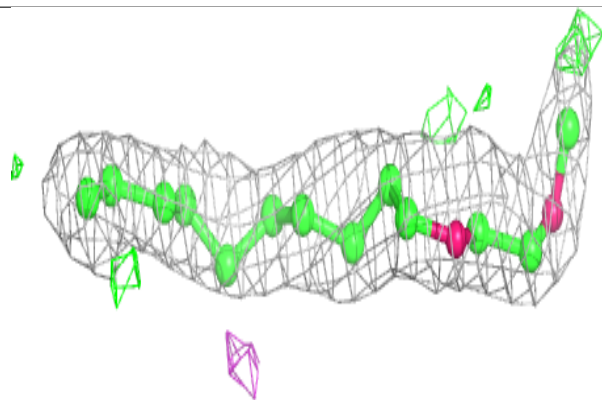
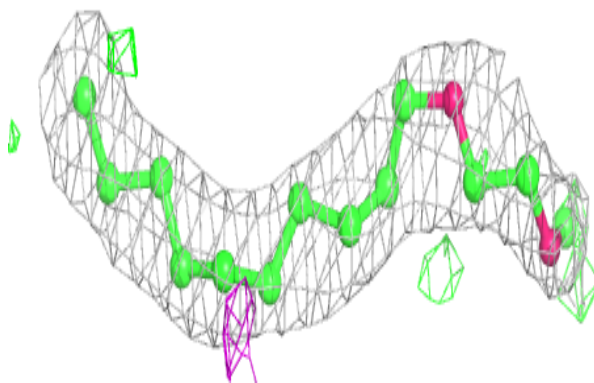
**Electron density around CXE A 514:**

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

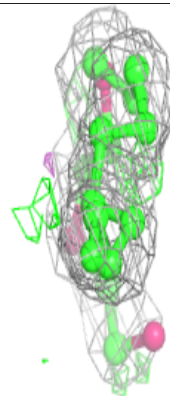
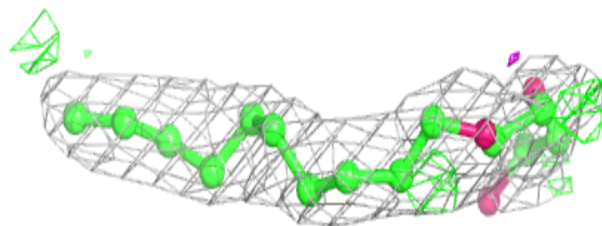
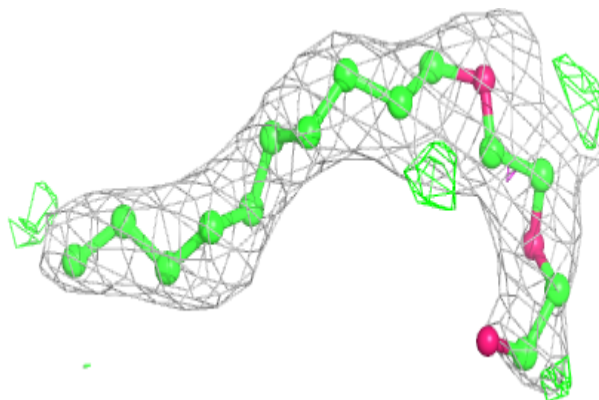


Electron density around CXE C 506:

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

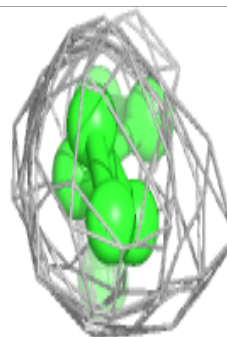
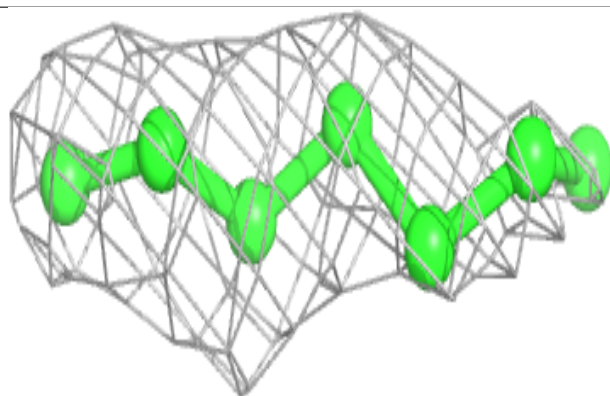
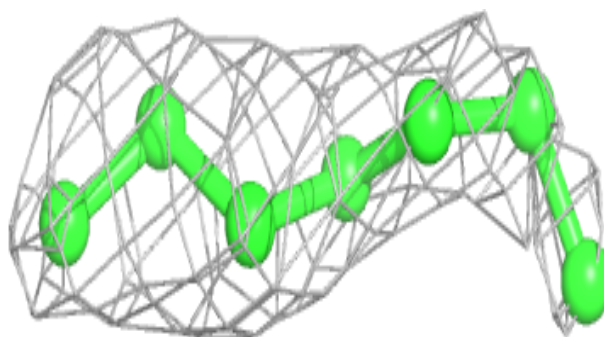
**Electron density around CXE B 503:**

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

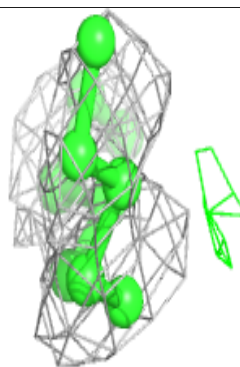
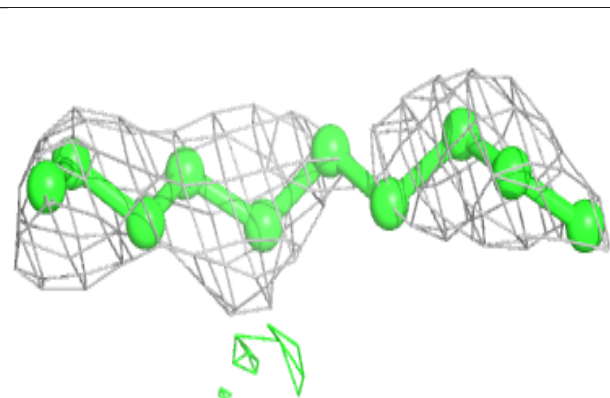
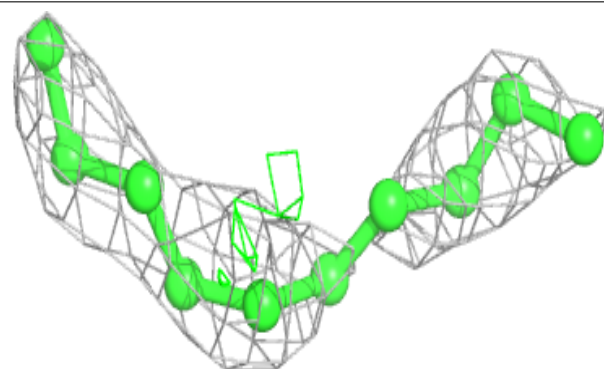


Electron density around CXE B 508:

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

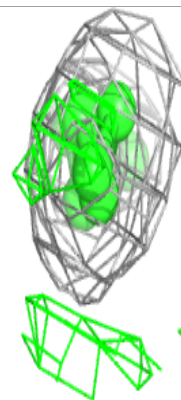
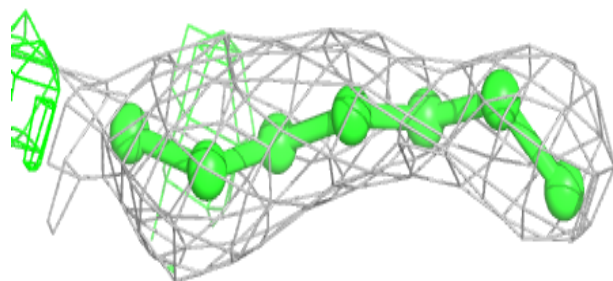
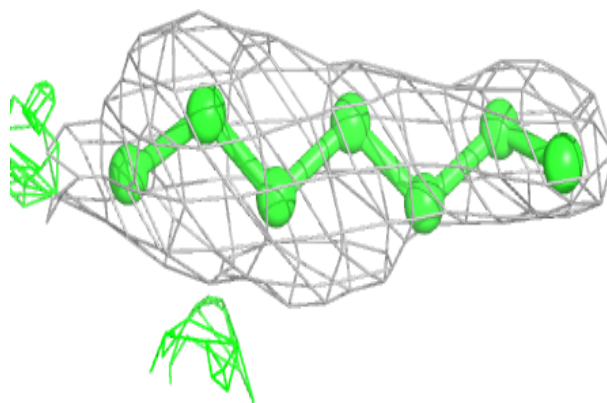
**Electron density around CXE C 507:**

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

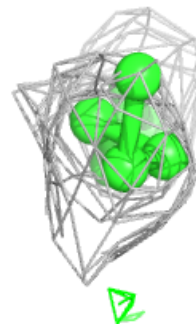
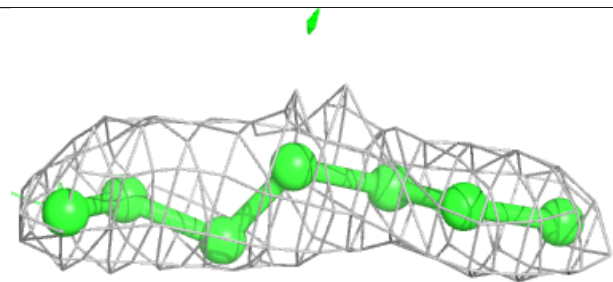
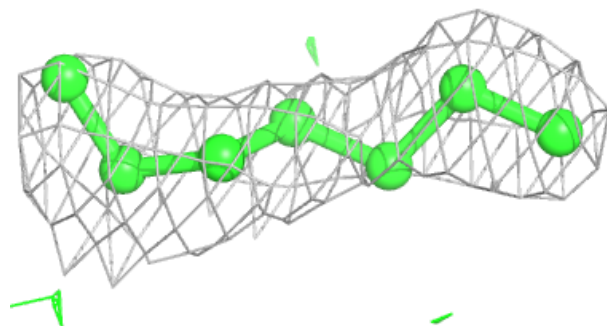


Electron density around CXE A 515:

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

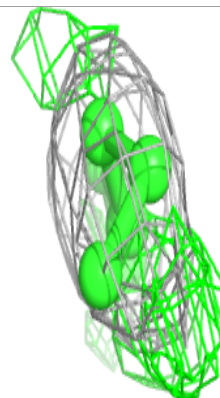
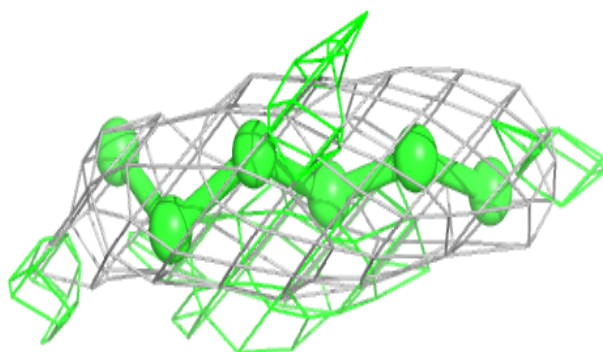
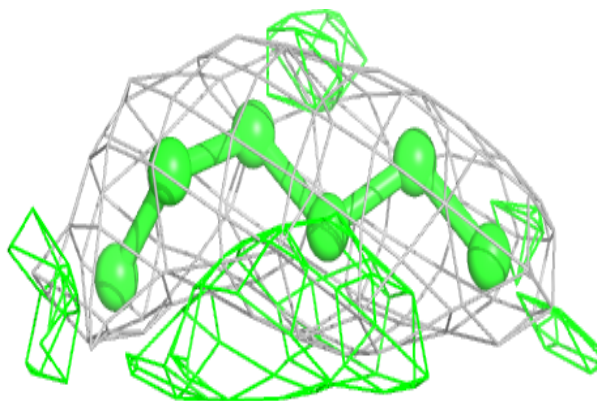
**Electron density around CXE C 516:**

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

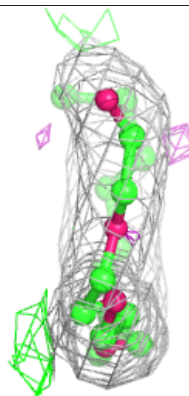
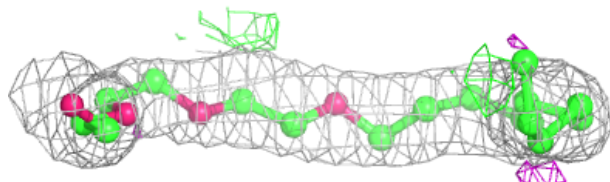
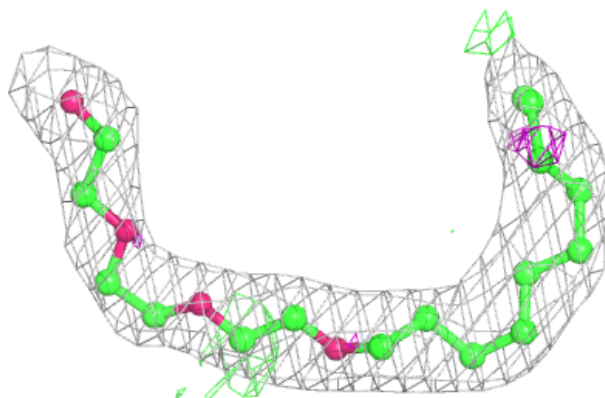


Electron density around CXE B 509:

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

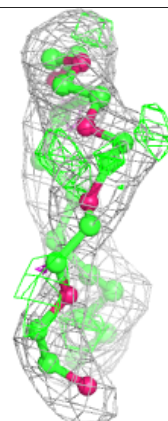
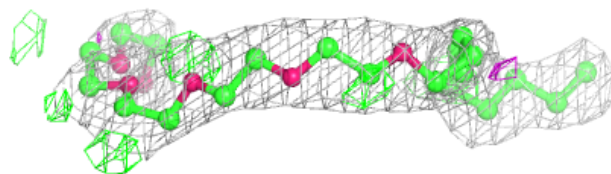
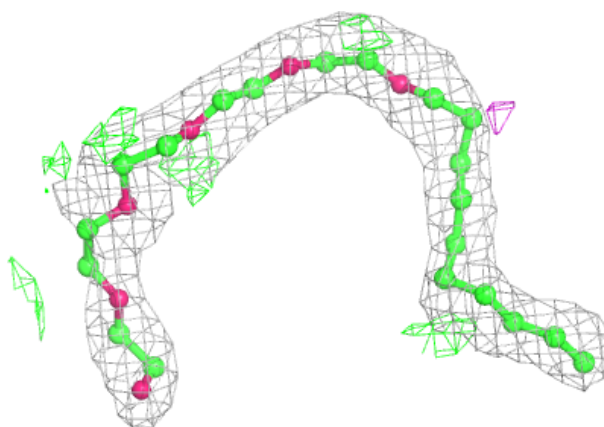
**Electron density around CXE A 506:**

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

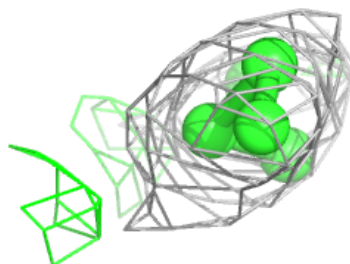
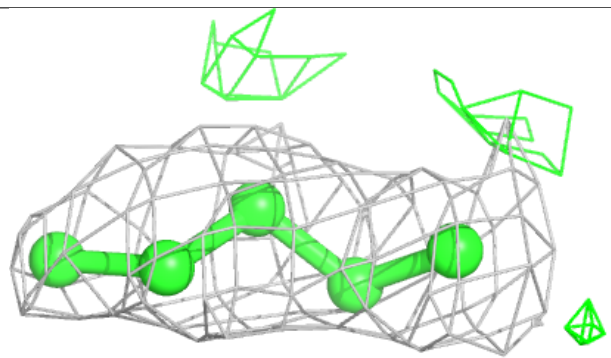
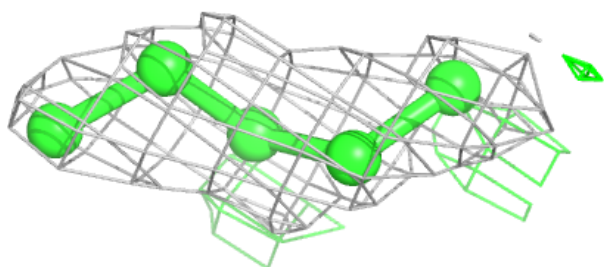


Electron density around CXE A 502:

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

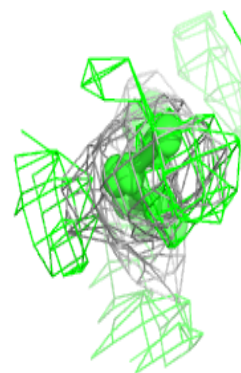
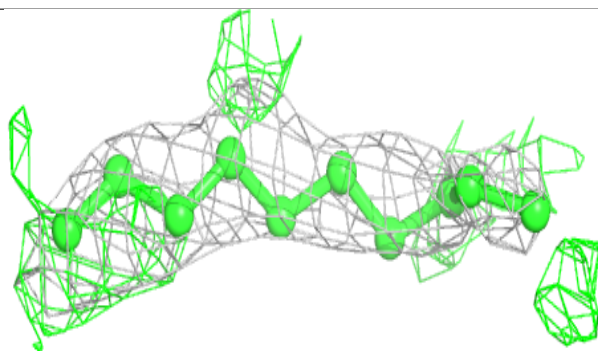
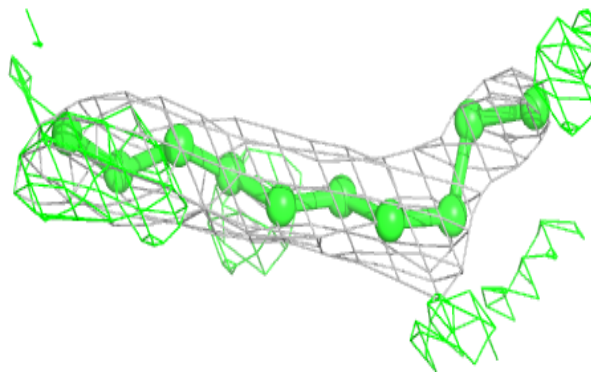
**Electron density around CXE A 517:**

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

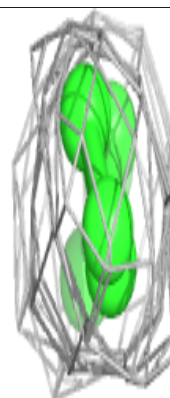
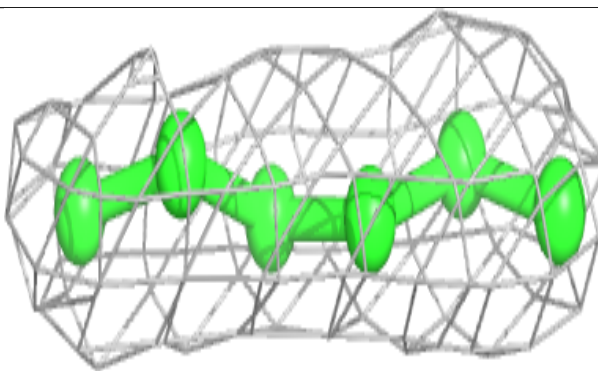
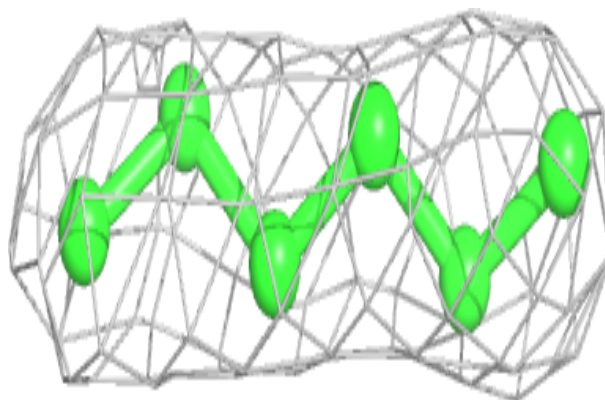


Electron density around CXE A 505:

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

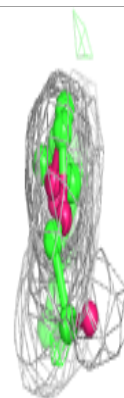
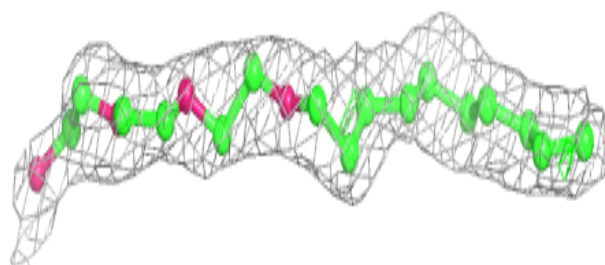
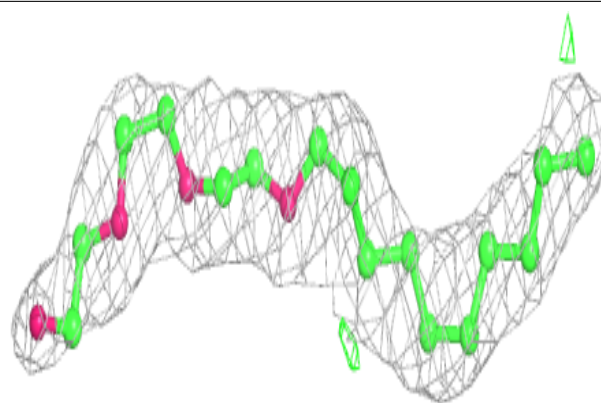
**Electron density around CXE B 510:**

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

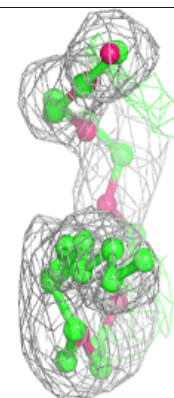
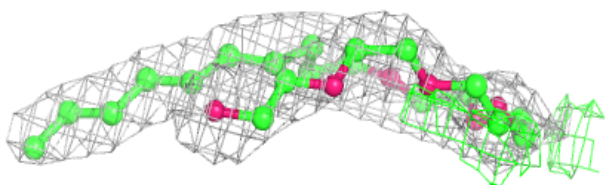
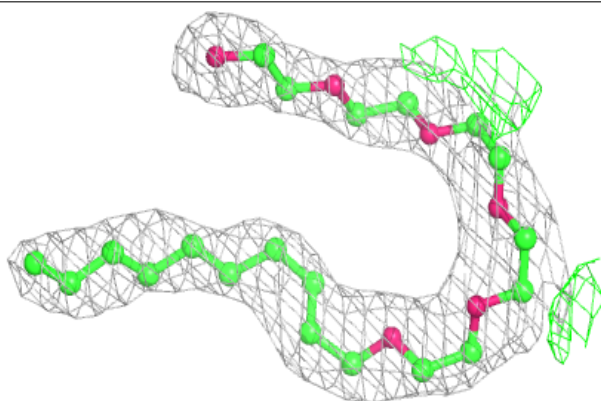


Electron density around CXE A 504:

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

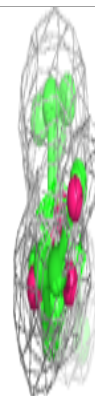
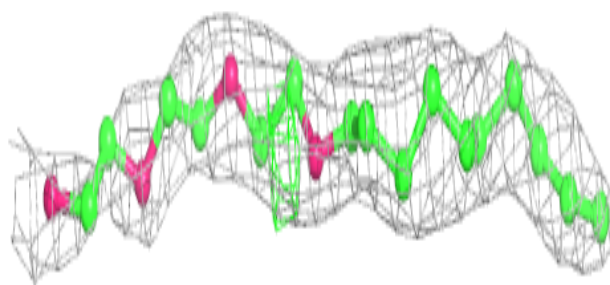
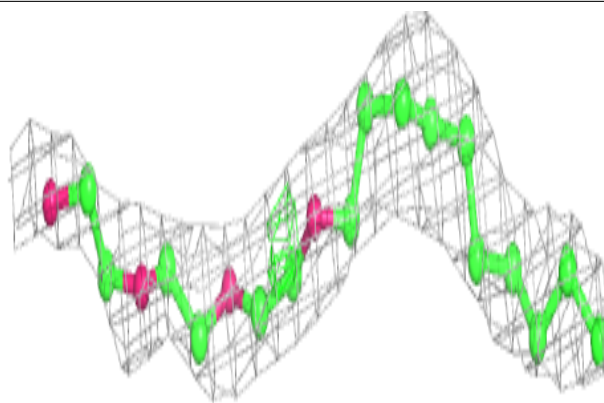
**Electron density around CXE B 501:**

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

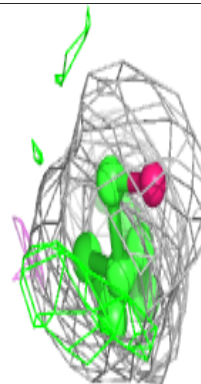
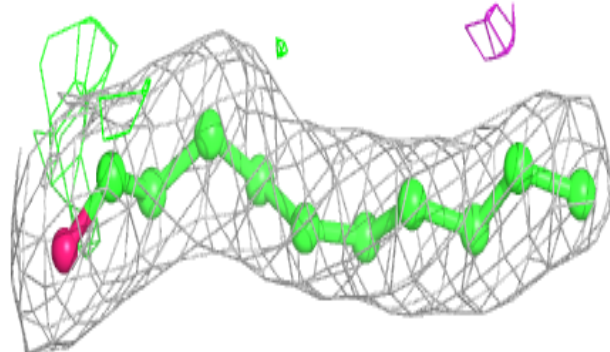
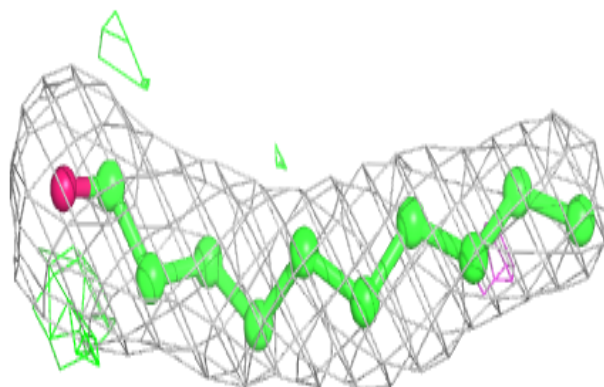


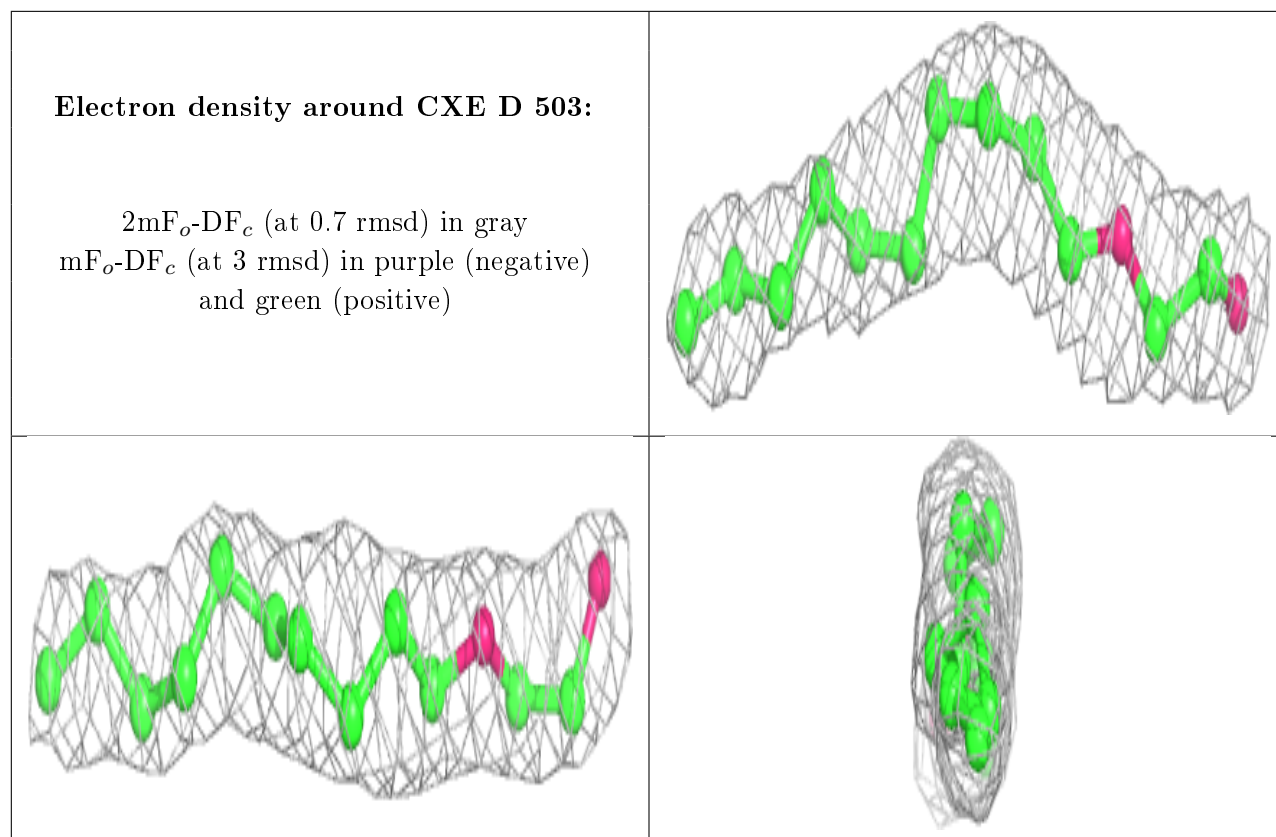
Electron density around CXE D 502:

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

**Electron density around CXE 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.