



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2024 – 06:28 AM EDT

PDB ID : 1MX9
Title : Crystal Structure of Human Liver Carboxylesterase in complexed with nalox-one methiodide, a heroin analogue
Authors : Bencharit, S.; Morton, C.L.; Xue, Y.; Potter, P.M.; Redinbo, M.R.
Deposited on : 2002-10-01
Resolution : 2.90 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

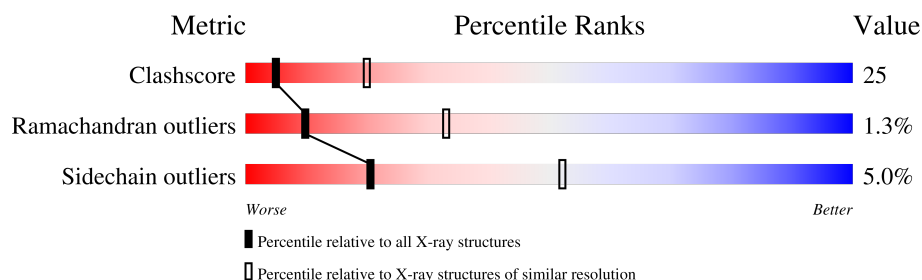
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	548	
1	B	548	
1	C	548	
1	D	548	
1	E	548	
1	F	548	
1	G	548	
1	H	548	

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Mol	Chain	Length	Quality of chain
1	I	548	
1	J	548	
1	K	548	
1	L	548	

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	NAG	J	479	-	-	X	-
3	NLX	A	1	X	-	X	-
3	NLX	B	2	X	-	X	-
3	NLX	C	3	X	-	X	-
3	NLX	D	4	X	-	X	-
3	NLX	E	5	X	-	X	-
3	NLX	F	6	X	-	X	-
3	NLX	G	1	X	-	X	-
3	NLX	H	2	X	-	X	-
3	NLX	I	3	X	-	X	-
3	NLX	J	4	X	-	X	-
3	NLX	K	5	X	-	X	-
3	NLX	L	6	X	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51134 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 liver Carboxylesterase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	B	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	C	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	D	533	Total	C	N	O	S	0	0	0
			4135	2665	686	764	20			
1	E	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	F	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	G	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	H	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	I	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	J	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	K	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	L	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			

There are 12 discrepancies between the modelled and reference sequences:

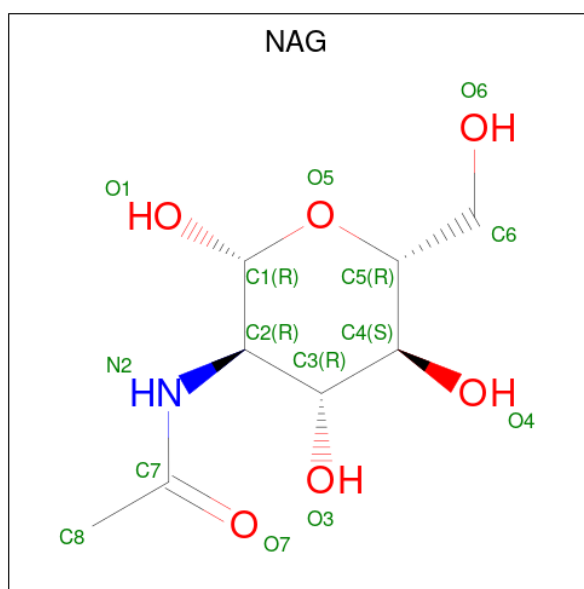
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P23141
B	?	-	GLN	deletion	UNP P23141
C	?	-	GLN	deletion	UNP P23141
D	?	-	GLN	deletion	UNP P23141
E	?	-	GLN	deletion	UNP P23141

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLN	deletion	UNP P23141
G	?	-	GLN	deletion	UNP P23141
H	?	-	GLN	deletion	UNP P23141
I	?	-	GLN	deletion	UNP P23141
J	?	-	GLN	deletion	UNP P23141
K	?	-	GLN	deletion	UNP P23141
L	?	-	GLN	deletion	UNP P23141

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



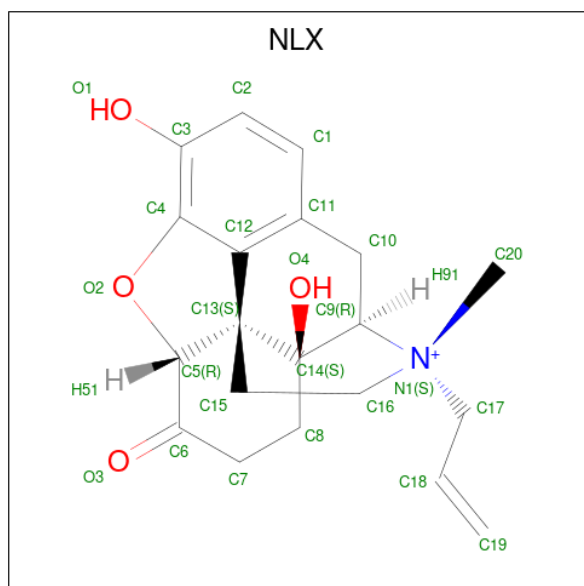
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	K	1	Total	C	N	O	0	0
			14	8	1	5		
2	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is (5A,17R)-4,5-EPOXY-3,14-DIHYDROXY-17-METHYL-6-OXO-17-(2-PROPENYL)-MORPHINANIUM (three-letter code: NLX) (formula: $C_{20}H_{24}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	20	1	4		
3	B	1	Total	C	N	O	0	0
			25	20	1	4		
3	C	1	Total	C	N	O	0	0
			25	20	1	4		
3	D	1	Total	C	N	O	0	0
			25	20	1	4		
3	E	1	Total	C	N	O	0	0
			25	20	1	4		

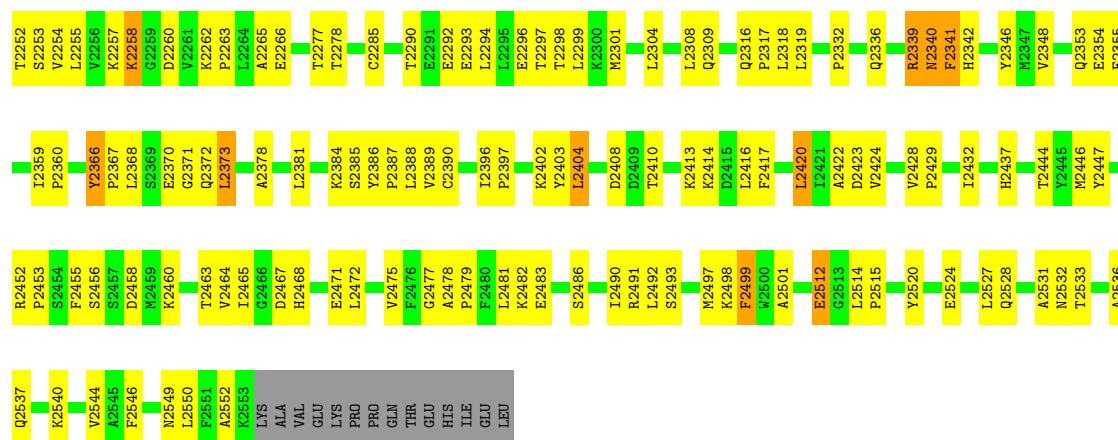
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			25	20	1	4		
3	G	1	Total	C	N	O	0	0
			25	20	1	4		
3	H	1	Total	C	N	O	0	0
			25	20	1	4		
3	I	1	Total	C	N	O	0	0
			25	20	1	4		
3	J	1	Total	C	N	O	0	0
			25	20	1	4		
3	K	1	Total	C	N	O	0	0
			25	20	1	4		
3	L	1	Total	C	N	O	0	0
			25	20	1	4		

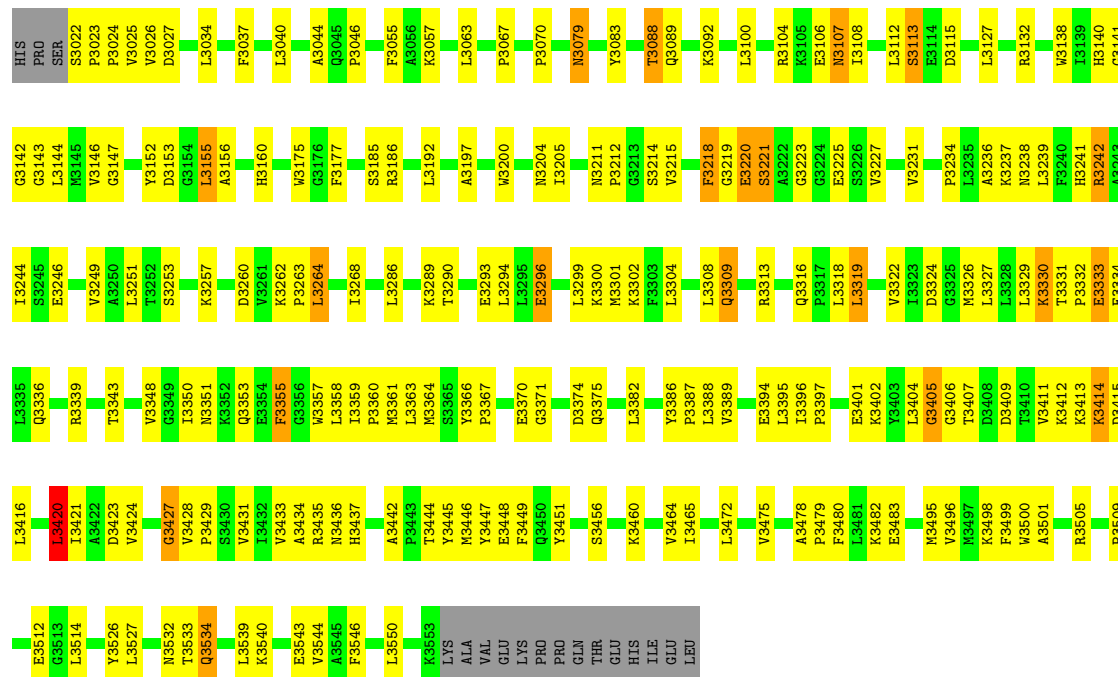
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	120	Total	O	0	0
			120	120		
4	C	98	Total	O	0	0
			98	98		
4	D	119	Total	O	0	0
			119	119		
4	E	112	Total	O	0	0
			112	112		
4	F	91	Total	O	0	0
			91	91		
4	G	69	Total	O	0	0
			69	69		
4	H	95	Total	O	0	0
			95	95		
4	I	80	Total	O	0	0
			80	80		
4	J	110	Total	O	0	0
			110	110		
4	K	73	Total	O	0	0
			73	73		
4	L	75	Total	O	0	0
			75	75		



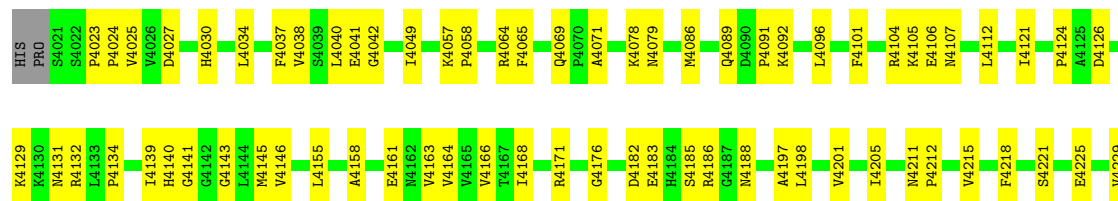
• Molecule 1: liver Carboxylesterase I

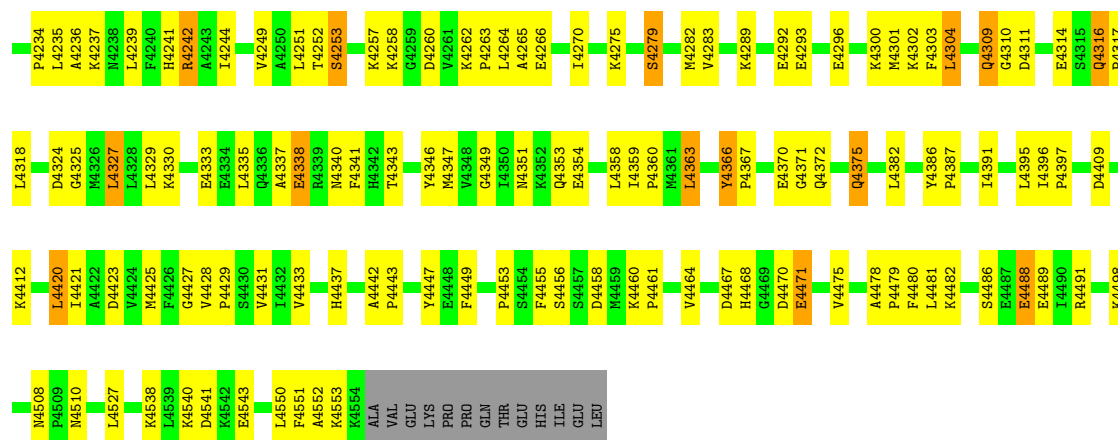
Chain C: 59% 34%



• Molecule 1: liver Carboxylesterase I

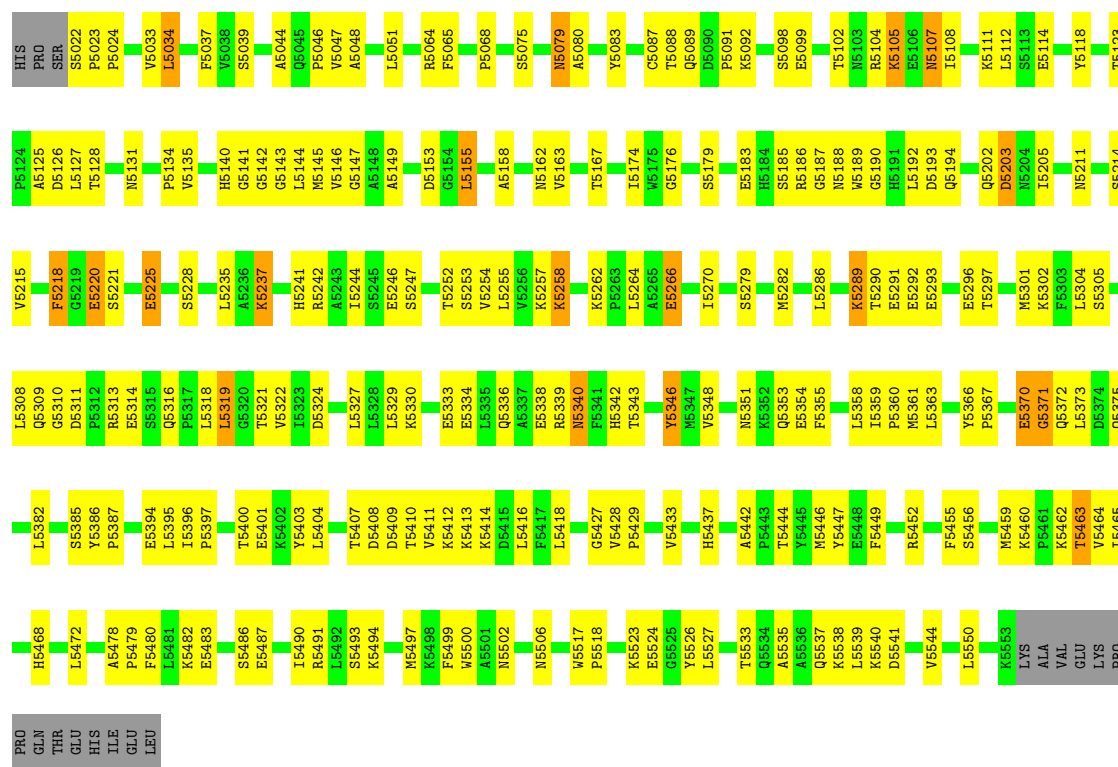
Chain D: 62% 33%





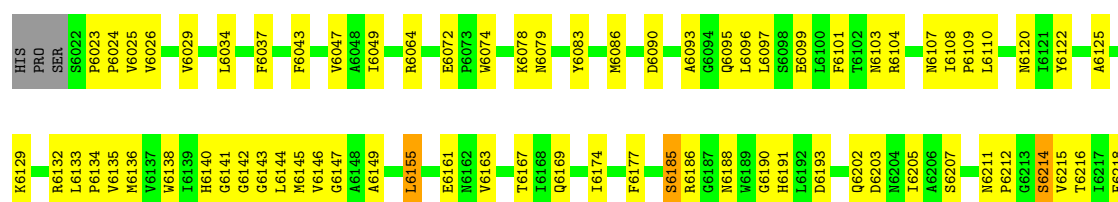
• Molecule 1: liver Carboxylesterase I

Chain E: 55% 38%

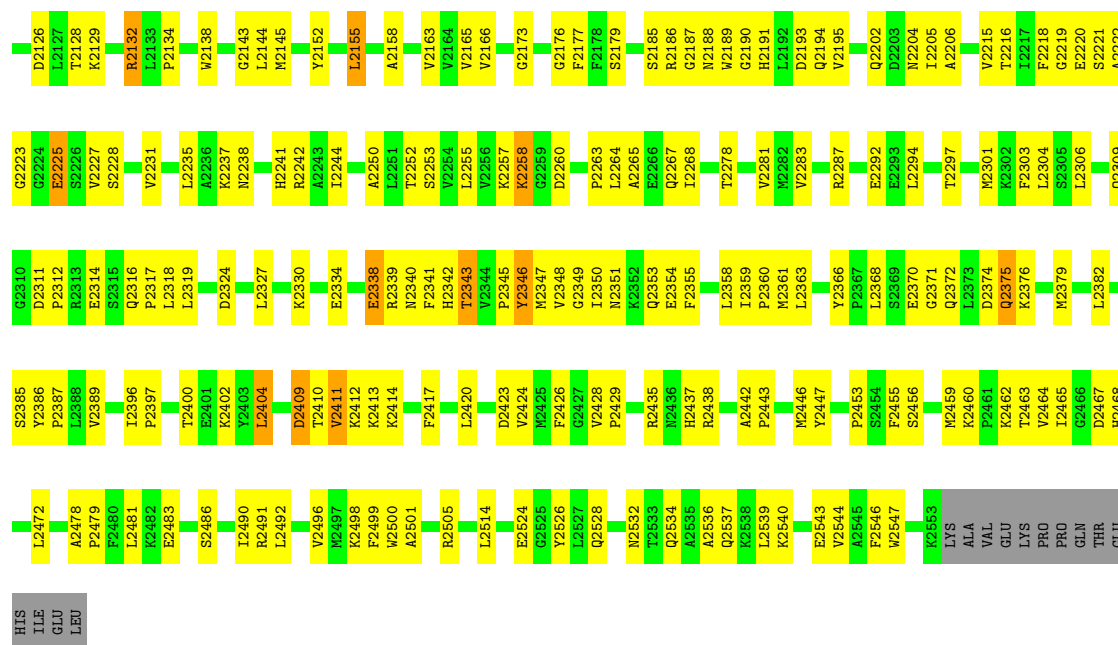


• Molecule 1: liver Carboxylesterase I

Chain F: 57% 37%

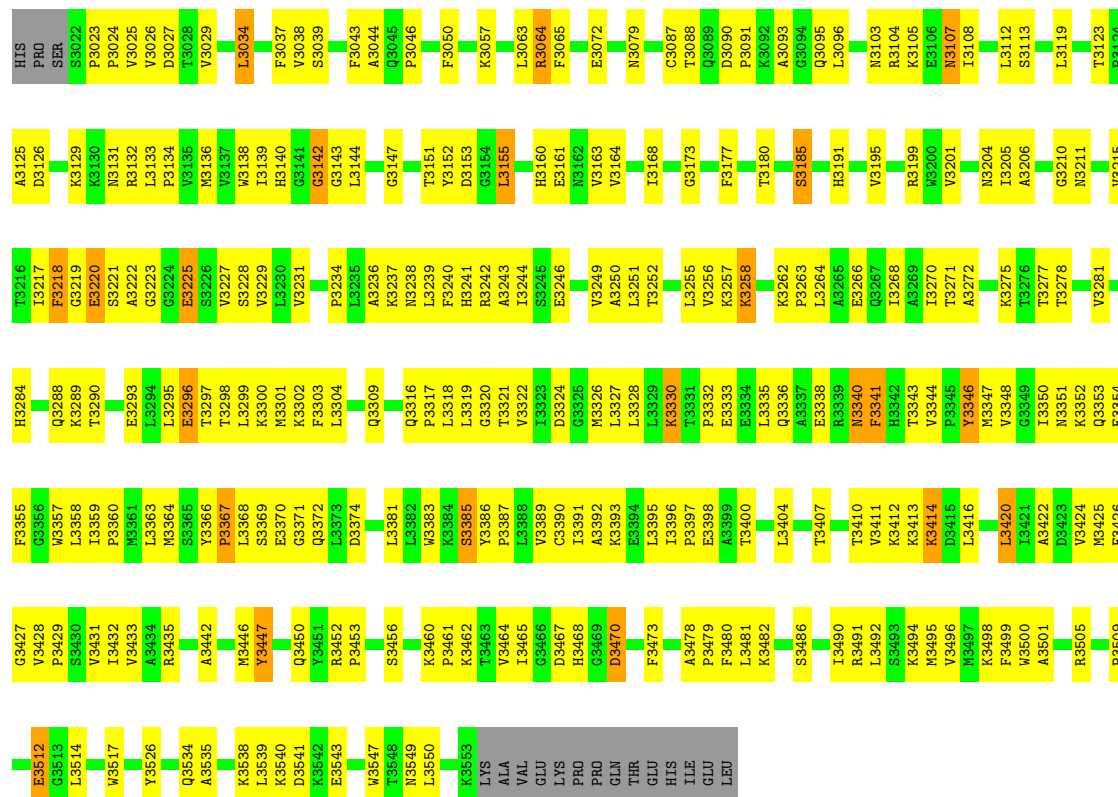




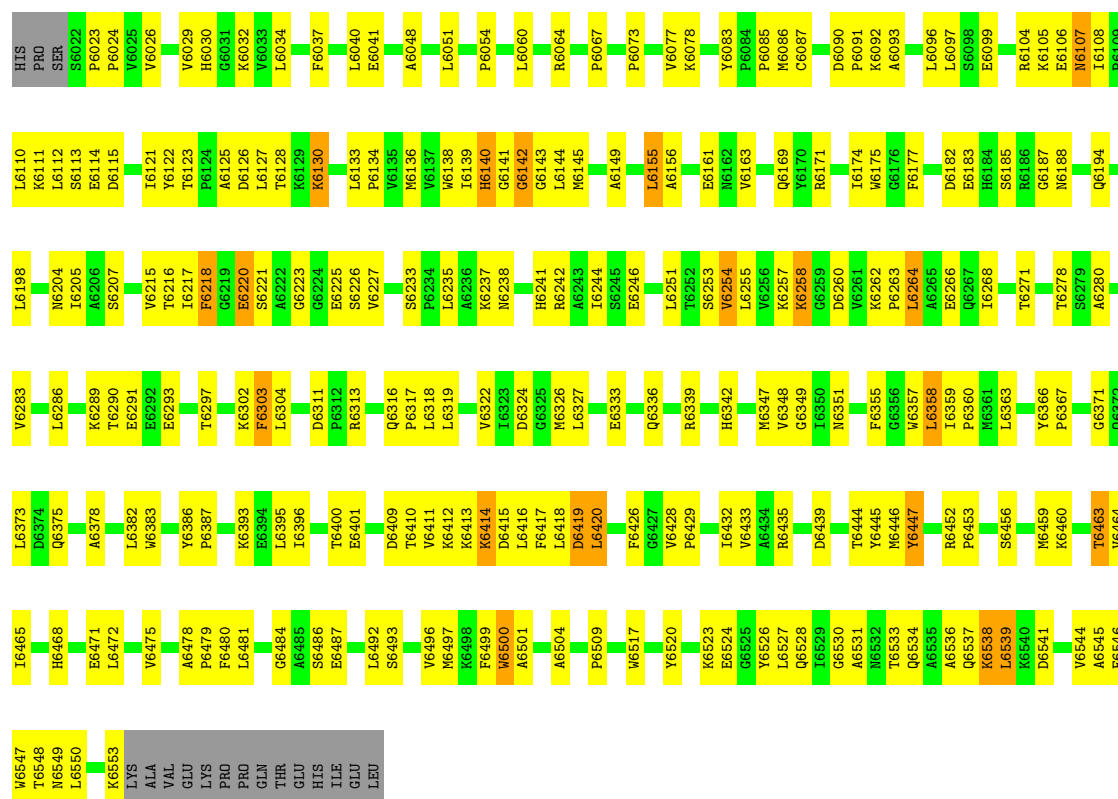


• Molecule 1: liver Carboxylesterase I

Chain I: 49% 43%



Response	Percentage
Yes	54%
No	40%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.17Å 120.71Å 177.02Å 90.28° 89.32° 99.22°	Depositor
Resolution (Å)	29.82 – 2.90	Depositor
% Data completeness (in resolution range)	95.7 (29.82-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.214 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	51134	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

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: NLX, NAG

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	0.38	0/4236	0.62	0/5754
1	B	0.41	0/4236	0.66	2/5754 (0.0%)
1	C	0.42	0/4230	0.65	2/5746 (0.0%)
1	D	0.41	0/4241	0.63	0/5761
1	E	0.40	0/4230	0.64	1/5746 (0.0%)
1	F	0.38	0/4230	0.62	0/5746
1	G	0.36	0/4236	0.60	0/5754
1	H	0.39	0/4230	0.63	0/5746
1	I	0.36	0/4230	0.61	0/5746
1	J	0.39	0/4236	0.62	0/5754
1	K	0.36	0/4230	0.60	0/5746
1	L	0.37	0/4230	0.63	1/5746 (0.0%)
All	All	0.39	0/50795	0.63	6/68999 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3420	LEU	CA-CB-CG	5.80	128.63	115.30
1	C	3388	LEU	CB-CG-CD2	-5.50	101.66	111.00
1	B	2339	ARG	N-CA-C	5.37	125.50	111.00
1	B	2075	SER	N-CA-C	5.33	125.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	6140	HIS	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	5118	TYR	Sidechain

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	4130	0	4132	231	0
1	B	4130	0	4132	182	0
1	C	4124	0	4127	180	0
1	D	4135	0	4134	165	0
1	E	4124	0	4127	200	0
1	F	4124	0	4127	192	0
1	G	4130	0	4132	237	0
1	H	4124	0	4127	194	0
1	I	4124	0	4127	232	0
1	J	4130	0	4134	216	0
1	K	4124	0	4127	226	0
1	L	4124	0	4127	244	0
2	A	28	0	26	3	0
2	B	14	0	13	4	0
2	C	14	0	13	0	0
2	D	14	0	13	4	0
2	E	14	0	13	2	0
2	F	14	0	13	0	0
2	G	14	0	13	4	0
2	H	14	0	13	1	0
2	I	14	0	13	1	0
2	J	14	0	13	7	0
2	K	14	0	13	1	0
2	L	14	0	13	0	0
3	A	25	0	23	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	23	21	0
3	C	25	0	19	27	0
3	D	25	0	24	15	0
3	E	25	0	24	18	0
3	F	25	0	21	23	0
3	G	25	0	23	12	0
3	H	25	0	23	30	0
3	I	25	0	24	19	0
3	J	25	0	24	20	0
3	K	25	0	24	18	0
3	L	25	0	24	23	0
4	A	87	0	0	9	0
4	B	120	0	0	12	0
4	C	98	0	0	10	0
4	D	119	0	0	9	0
4	E	112	0	0	16	0
4	F	91	0	0	8	0
4	G	69	0	0	10	0
4	H	95	0	0	10	0
4	I	80	0	0	10	0
4	J	110	0	0	8	0
4	K	73	0	0	11	0
4	L	75	0	0	15	0
All	All	51134	0	49998	2453	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 25.

The worst 5 of 2453 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)
3:C:3:NLX:N1	3:C:3:NLX:C9	1.69	1.56
3:C:3:NLX:C9	3:C:3:NLX:C14	1.78	1.55
1:D:4343:THR:HB	1:D:4442:ALA:HB2	1.17	1.13
1:H:2304:LEU:HB3	3:H:2:NLX:H201	1.28	1.11
1:C:3364:MET:CE	3:C:3:NLX:H181	1.83	1.08

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	530/548 (97%)	480 (91%)	41 (8%)	9 (2%)	7	27
1	B	530/548 (97%)	476 (90%)	48 (9%)	6 (1%)	12	37
1	C	529/548 (96%)	489 (92%)	33 (6%)	7 (1%)	10	33
1	D	531/548 (97%)	491 (92%)	36 (7%)	4 (1%)	16	45
1	E	529/548 (96%)	482 (91%)	40 (8%)	7 (1%)	10	33
1	F	529/548 (96%)	477 (90%)	44 (8%)	8 (2%)	8	29
1	G	530/548 (97%)	467 (88%)	55 (10%)	8 (2%)	8	29
1	H	529/548 (96%)	470 (89%)	52 (10%)	7 (1%)	10	33
1	I	529/548 (96%)	466 (88%)	56 (11%)	7 (1%)	10	33
1	J	530/548 (97%)	484 (91%)	40 (8%)	6 (1%)	12	37
1	K	529/548 (96%)	475 (90%)	48 (9%)	6 (1%)	12	37
1	L	529/548 (96%)	467 (88%)	53 (10%)	9 (2%)	7	27
All	All	6354/6576 (97%)	5724 (90%)	546 (9%)	84 (1%)	10	33

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1253	SER
1	B	2342	HIS
1	C	3253	SER
1	D	4185	SER
1	D	4253	SER

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	448/463 (97%)	435 (97%)	13 (3%)	37	72
1	B	448/463 (97%)	431 (96%)	17 (4%)	28	63
1	C	447/463 (96%)	420 (94%)	27 (6%)	16	44
1	D	448/463 (97%)	423 (94%)	25 (6%)	17	47
1	E	447/463 (96%)	422 (94%)	25 (6%)	17	47
1	F	447/463 (96%)	426 (95%)	21 (5%)	22	55
1	G	448/463 (97%)	419 (94%)	29 (6%)	14	40
1	H	447/463 (96%)	427 (96%)	20 (4%)	23	56
1	I	447/463 (96%)	418 (94%)	29 (6%)	14	40
1	J	448/463 (97%)	426 (95%)	22 (5%)	21	53
1	K	447/463 (96%)	421 (94%)	26 (6%)	17	46
1	L	447/463 (96%)	433 (97%)	14 (3%)	35	70
All	All	5369/5556 (97%)	5101 (95%)	268 (5%)	20	52

5 of 268 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	5128	THR
1	K	5299	LEU
1	L	6264	LEU
1	E	5319	LEU
1	E	5266	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 177 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	2267	GLN
1	J	4238	ASN
1	H	2372	GLN
1	I	3336	GLN
1	J	4375	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	I	379	-	14,14,15	0.47	0	17,19,21	0.82	1 (5%)
3	NLX	J	4	-	26,29,29	3.49	14 (53%)	44,49,49	1.98	12 (27%)
2	NAG	B	279	-	14,14,15	0.50	0	17,19,21	0.61	0
3	NLX	E	5	-	26,29,29	3.13	16 (61%)	44,49,49	2.01	13 (29%)
2	NAG	A	180	-	14,14,15	0.61	0	17,19,21	0.68	0
2	NAG	A	179	-	14,14,15	0.66	0	17,19,21	0.68	0
3	NLX	I	3	-	26,29,29	3.22	17 (65%)	44,49,49	2.33	14 (31%)
3	NLX	F	6	-	26,29,29	3.44	18 (69%)	44,49,49	4.85	23 (52%)
2	NAG	H	279	-	14,14,15	0.49	0	17,19,21	0.68	0
2	NAG	G	179	-	14,14,15	0.57	0	17,19,21	0.60	0
2	NAG	E	579	-	14,14,15	0.52	0	17,19,21	0.80	1 (5%)
2	NAG	C	379	-	14,14,15	0.48	0	17,19,21	0.76	0
3	NLX	G	1	-	26,29,29	3.47	15 (57%)	44,49,49	2.19	12 (27%)
2	NAG	D	479	-	14,14,15	0.45	0	17,19,21	0.64	0
2	NAG	F	679	-	14,14,15	0.51	0	17,19,21	0.79	1 (5%)
3	NLX	C	3	-	26,29,29	4.49	17 (65%)	44,49,49	4.63	18 (40%)
2	NAG	J	479	-	14,14,15	0.56	0	17,19,21	0.67	0
3	NLX	L	6	-	26,29,29	3.42	16 (61%)	44,49,49	2.15	13 (29%)
3	NLX	K	5	-	26,29,29	3.23	14 (53%)	44,49,49	2.05	12 (27%)
2	NAG	L	679	-	14,14,15	0.62	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	K	579	-	14,14,15	0.53	0	17,19,21	0.78	1 (5%)
3	NLX	D	4	-	26,29,29	3.37	16 (61%)	44,49,49	2.23	13 (29%)
3	NLX	H	2	-	26,29,29	3.35	15 (57%)	44,49,49	2.41	12 (27%)
3	NLX	B	2	-	26,29,29	3.01	15 (57%)	44,49,49	2.03	11 (25%)
3	NLX	A	1	-	26,29,29	3.76	15 (57%)	44,49,49	2.14	15 (34%)

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	NAG	I	379	-	-	4/6/23/26	0/1/1/1
3	NLX	J	4	-	1/1/6/7	0/4/62/62	0/6/5/5
2	NAG	B	279	-	-	2/6/23/26	0/1/1/1
3	NLX	E	5	-	1/1/6/7	0/4/62/62	0/6/5/5
2	NAG	A	180	-	-	2/6/23/26	0/1/1/1
2	NAG	A	179	-	-	4/6/23/26	0/1/1/1
3	NLX	I	3	-	1/1/6/7	1/4/62/62	0/6/5/5
3	NLX	F	6	-	1/1/6/7	2/4/62/62	0/6/5/5
2	NAG	H	279	-	-	4/6/23/26	0/1/1/1
2	NAG	G	179	-	-	5/6/23/26	0/1/1/1
2	NAG	E	579	-	-	0/6/23/26	0/1/1/1
2	NAG	C	379	-	-	2/6/23/26	0/1/1/1
3	NLX	G	1	-	1/1/6/7	1/4/62/62	0/6/5/5
2	NAG	D	479	-	-	2/6/23/26	0/1/1/1
2	NAG	F	679	-	-	3/6/23/26	0/1/1/1
3	NLX	C	3	-	1/1/6/7	1/4/62/62	0/6/5/5
2	NAG	J	479	-	-	4/6/23/26	0/1/1/1
3	NLX	L	6	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	K	5	-	1/1/6/7	0/4/62/62	0/6/5/5
2	NAG	L	679	-	-	2/6/23/26	0/1/1/1
2	NAG	K	579	-	-	4/6/23/26	0/1/1/1
3	NLX	D	4	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	H	2	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	B	2	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	A	1	-	1/1/6/7	0/4/62/62	0/6/5/5

The worst 5 of 188 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	NLX	C14-C9	15.46	1.78	1.55
3	D	4	NLX	C14-C9	10.69	1.71	1.55
3	H	2	NLX	C14-C9	10.43	1.71	1.55
3	J	4	NLX	C14-C9	10.06	1.70	1.55
3	A	1	NLX	C14-C9	9.94	1.70	1.55

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	NLX	C20-N1-C17	-19.90	63.74	107.94
3	F	6	NLX	C20-N1-C17	-18.82	66.14	107.94
3	C	3	NLX	C20-N1-C16	-15.60	68.71	108.71
3	F	6	NLX	C20-N1-C16	-14.40	71.79	108.71
3	F	6	NLX	O2-C5-C6	10.12	116.90	108.51

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1	NLX	N1
3	B	2	NLX	N1
3	C	3	NLX	N1
3	D	4	NLX	N1
3	E	5	NLX	N1

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	179	NAG	C8-C7-N2-C2
2	A	179	NAG	O7-C7-N2-C2
2	A	180	NAG	C8-C7-N2-C2
2	A	180	NAG	O7-C7-N2-C2
2	B	279	NAG	C8-C7-N2-C2

There are no ring outliers.

22 monomers are involved in 273 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	379	NAG	1	0
3	J	4	NLX	20	0
2	B	279	NAG	4	0
3	E	5	NLX	18	0

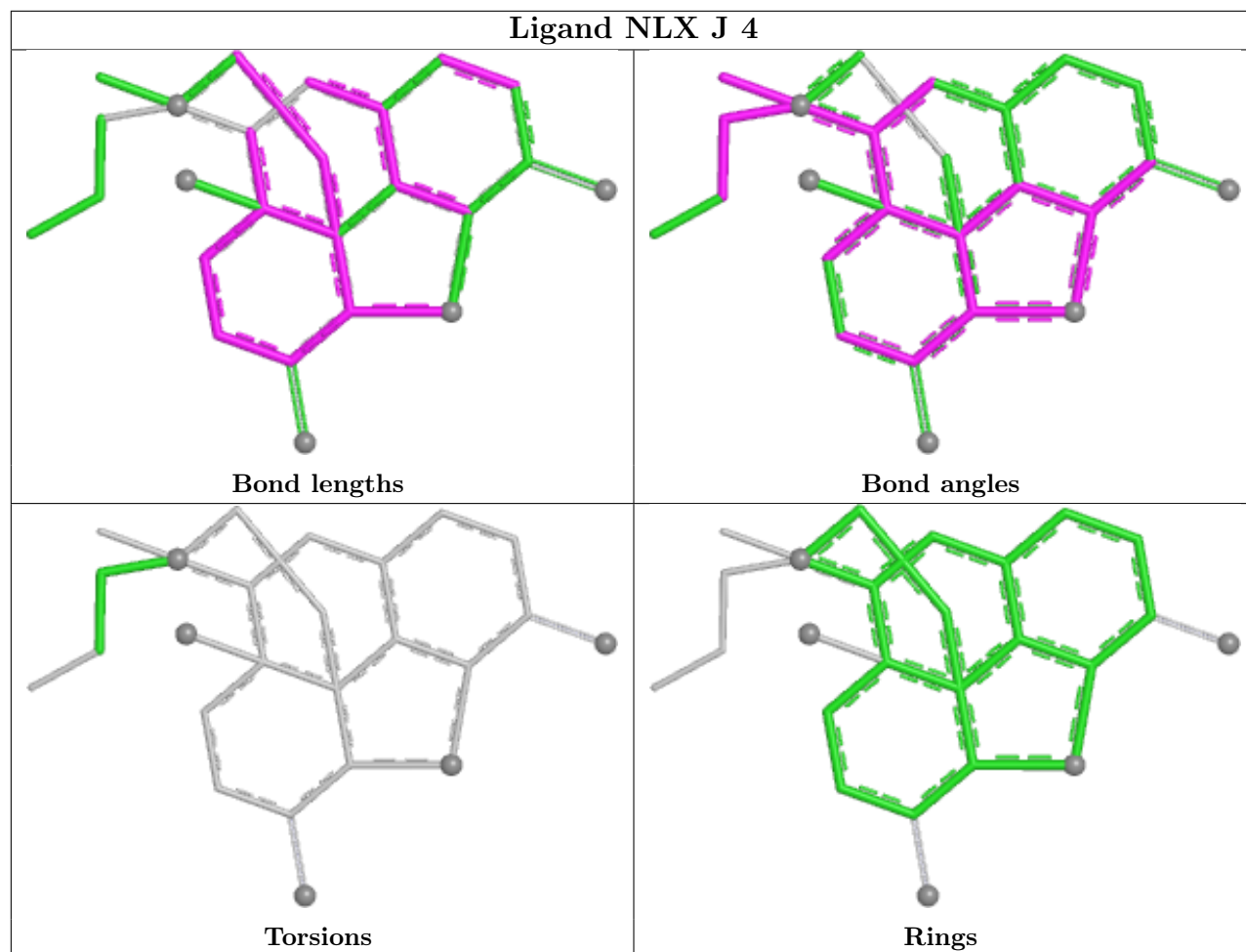
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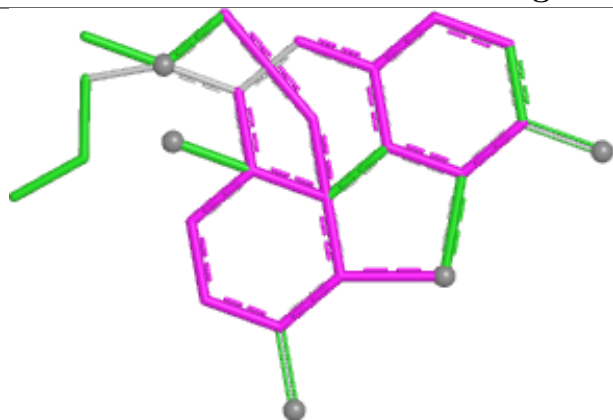
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	180	NAG	1	0
2	A	179	NAG	3	0
3	I	3	NLX	19	0
3	F	6	NLX	23	0
2	H	279	NAG	1	0
2	G	179	NAG	4	0
2	E	579	NAG	2	0
3	G	1	NLX	12	0
2	D	479	NAG	4	0
3	C	3	NLX	27	0
2	J	479	NAG	7	0
3	L	6	NLX	23	0
3	K	5	NLX	18	0
2	K	579	NAG	1	0
3	D	4	NLX	15	0
3	H	2	NLX	30	0
3	B	2	NLX	21	0
3	A	1	NLX	20	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.

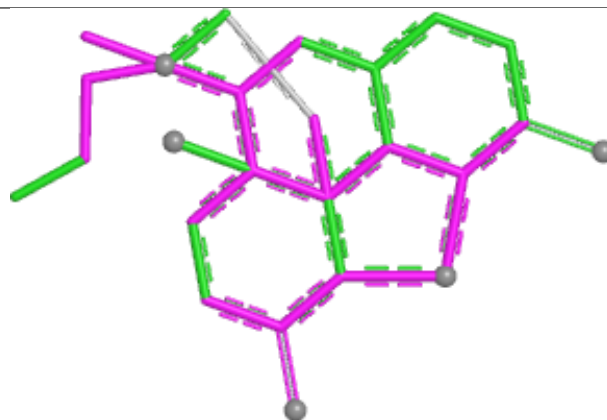
Ligand NLX J 4



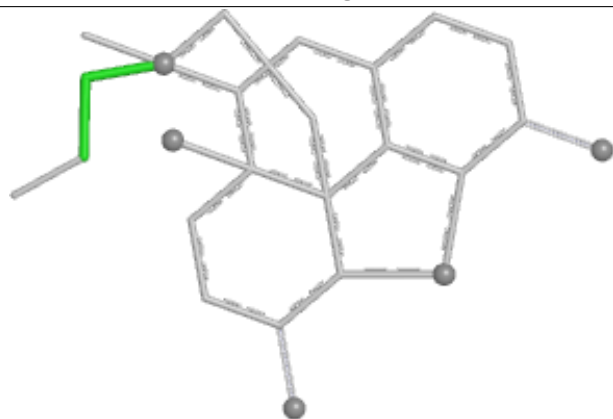
Ligand NLX E 5



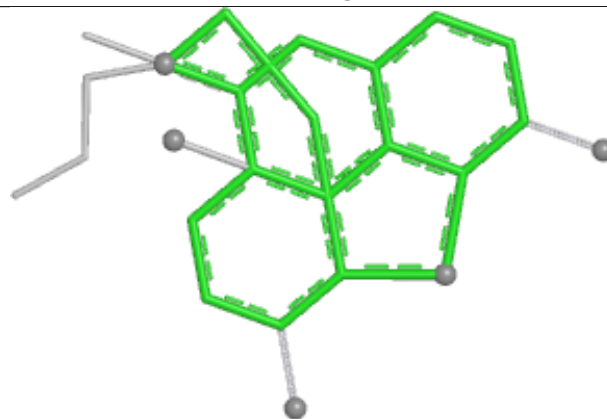
Bond lengths



Bond angles

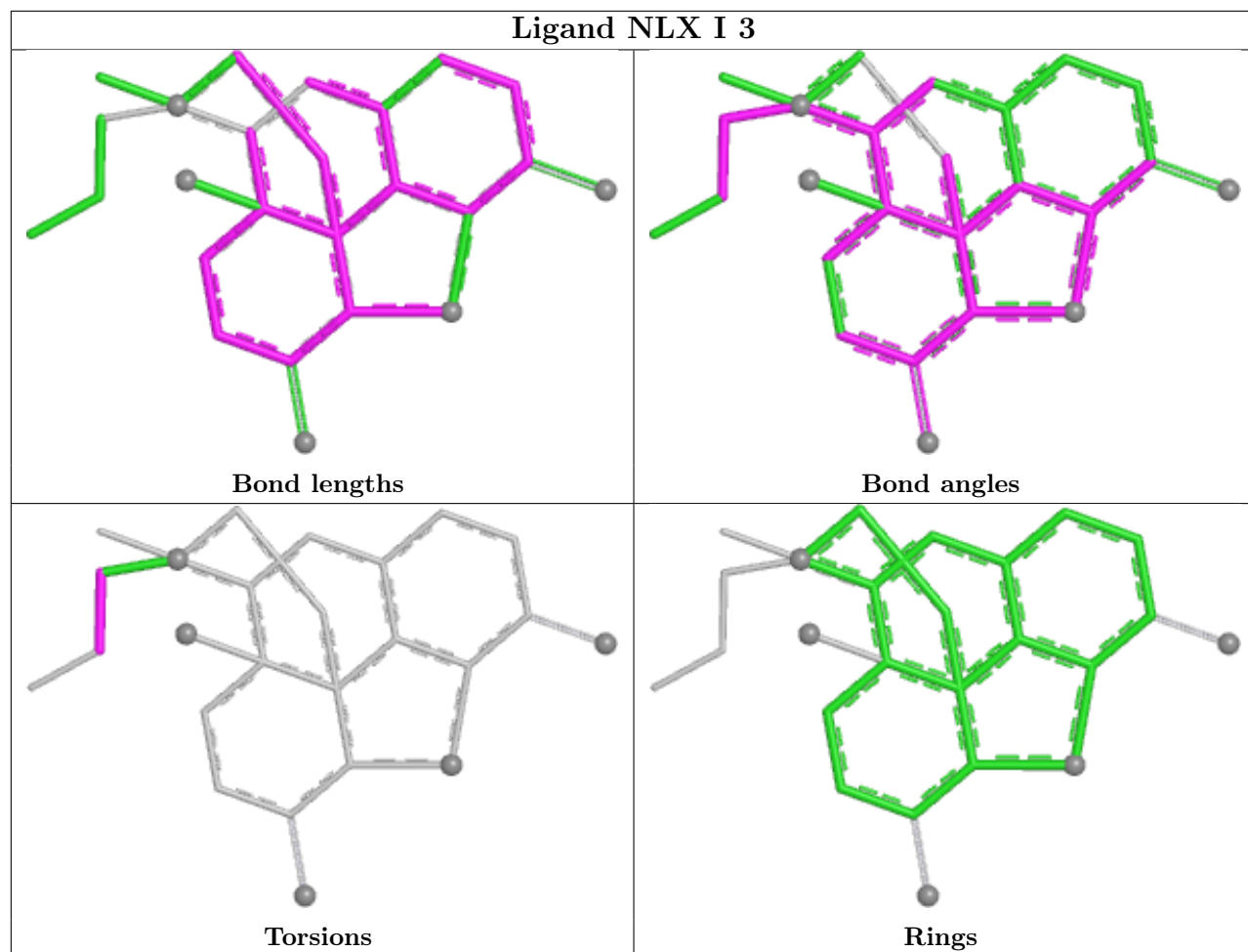


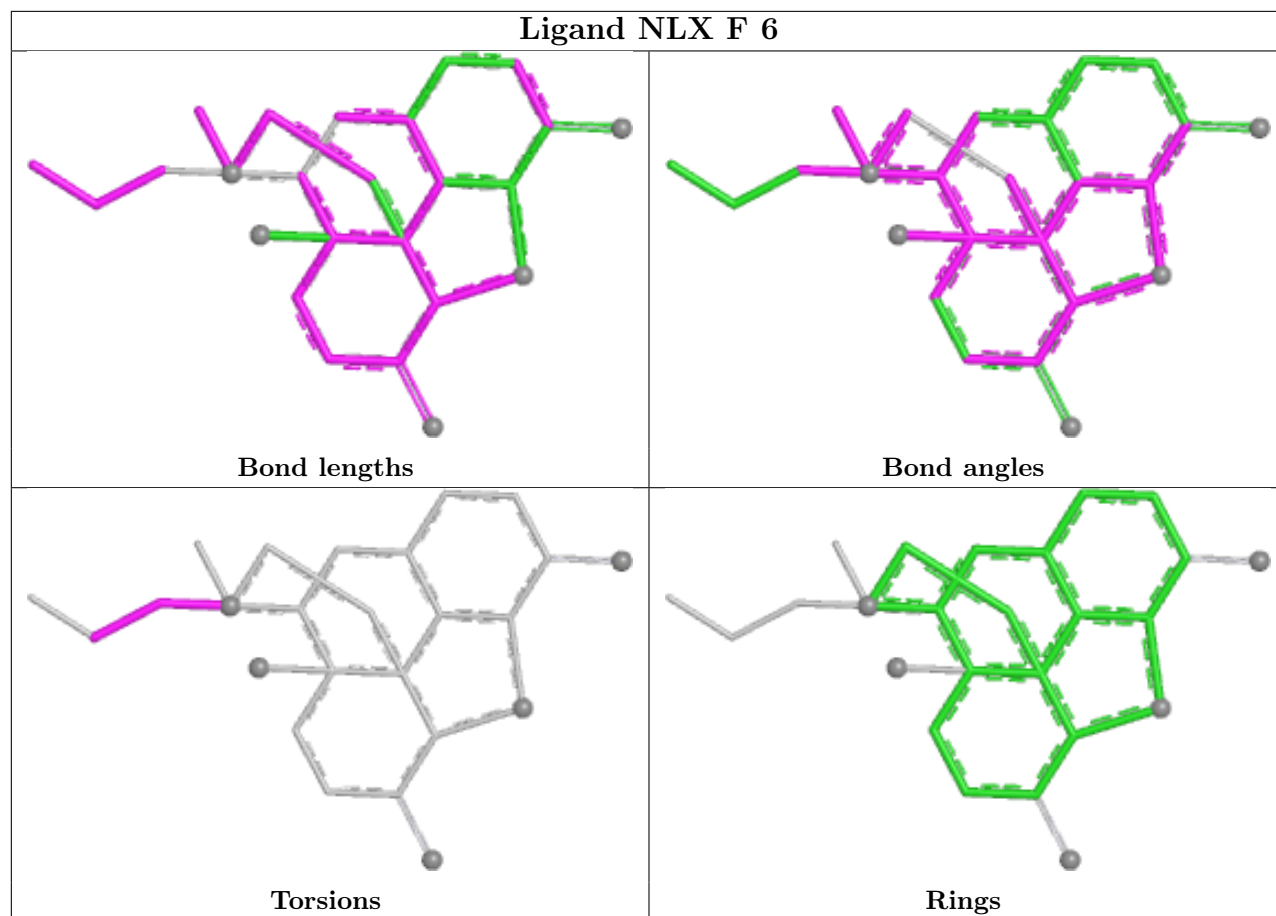
Torsions



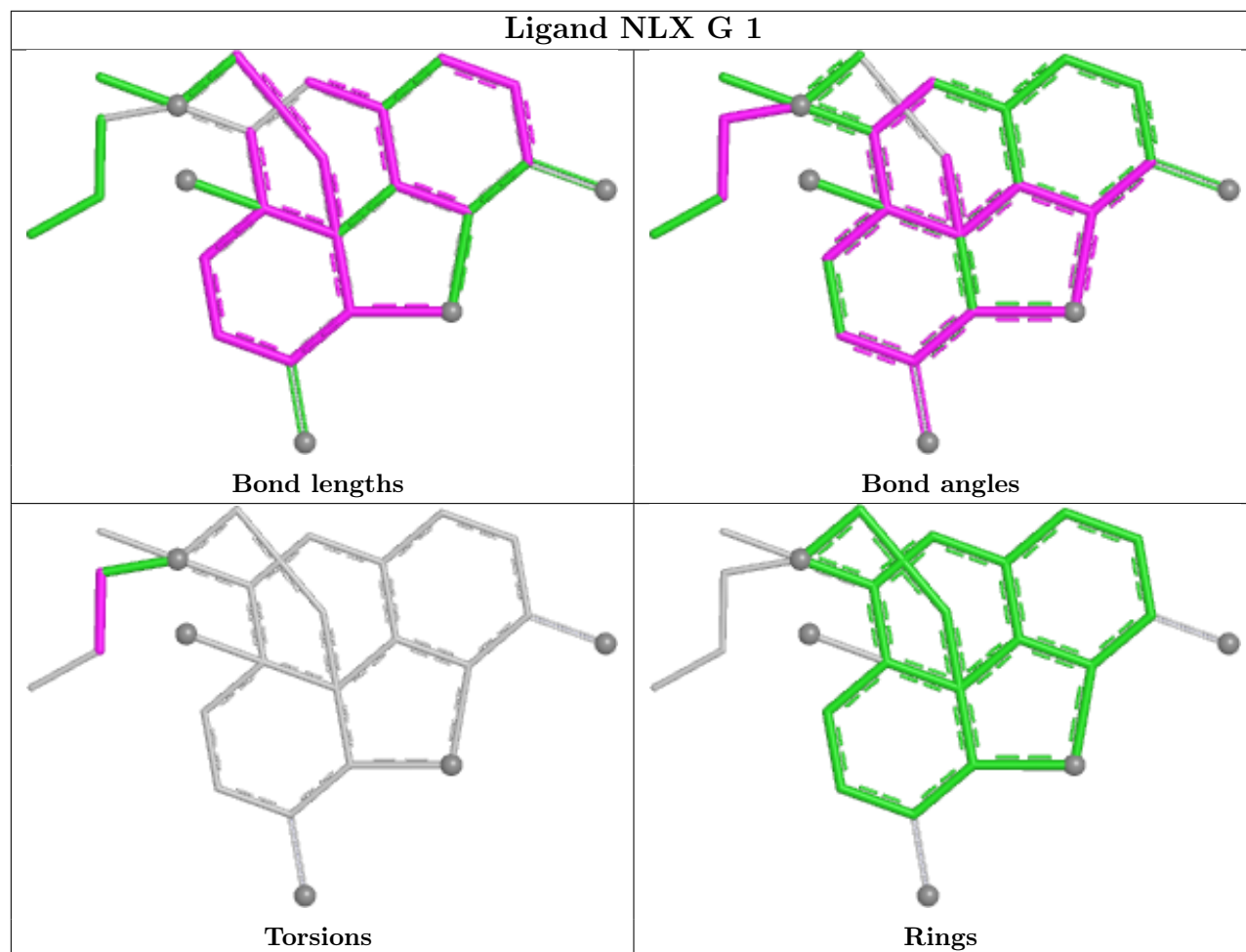
Rings

Ligand NLX I 3

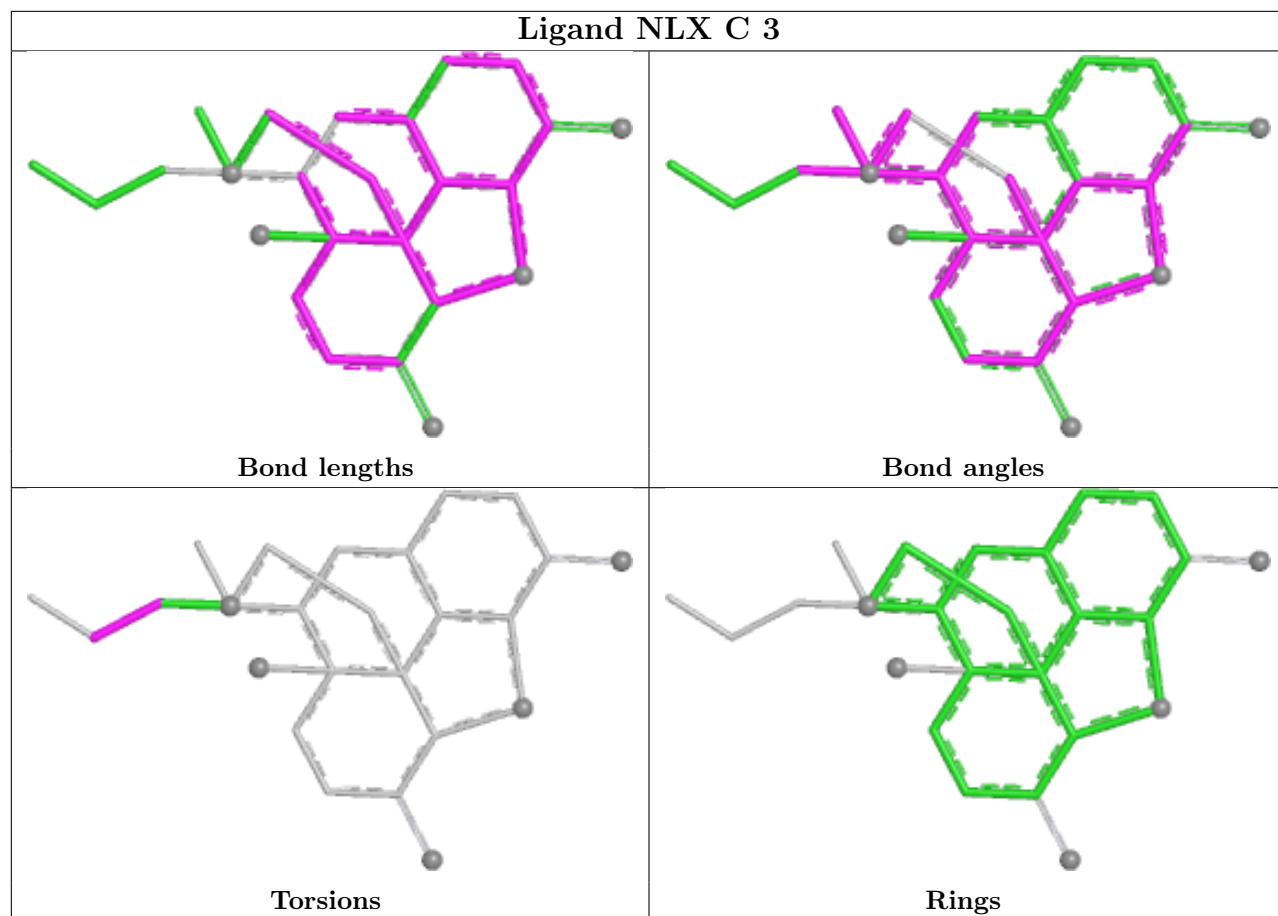




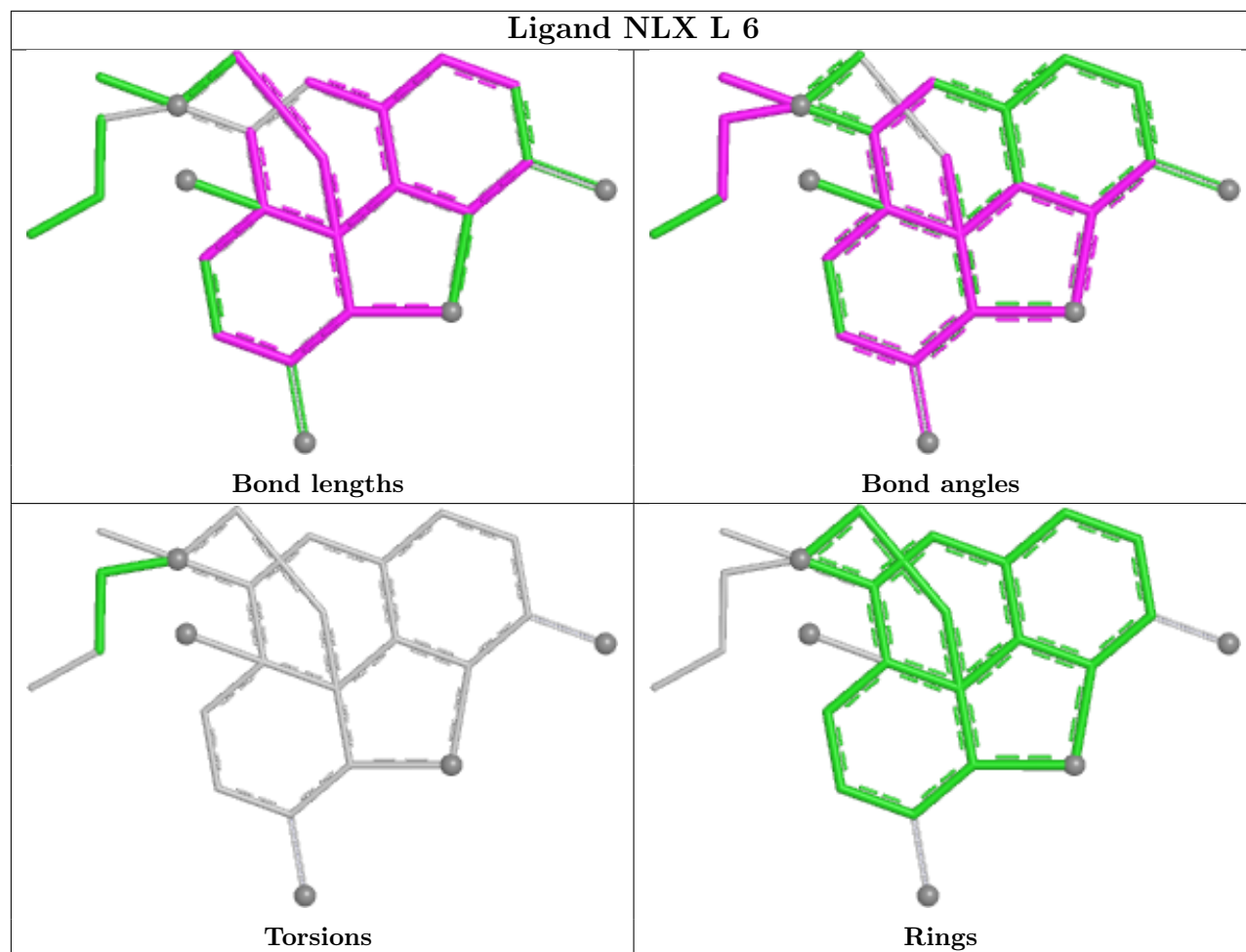
Ligand NLX G 1



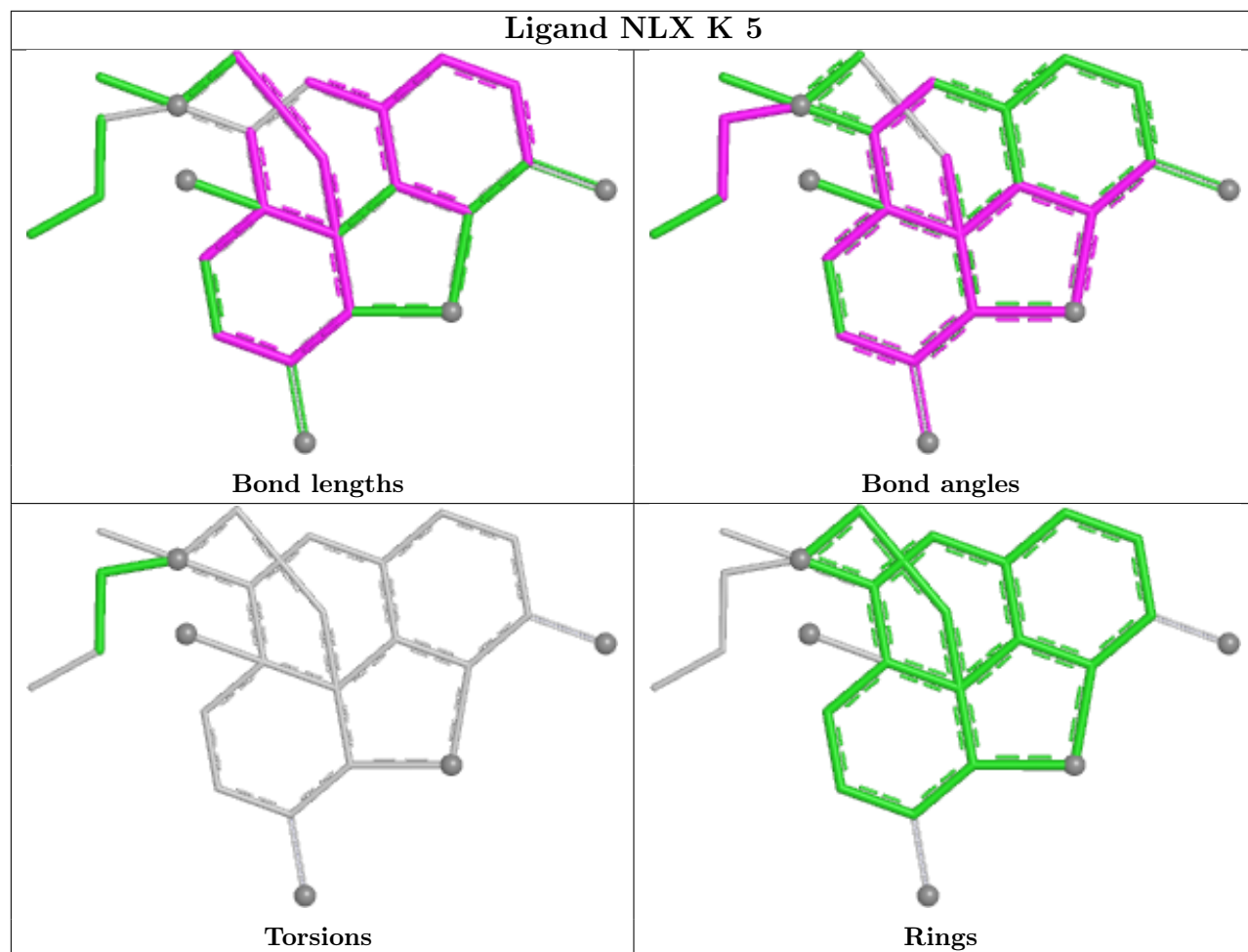
Ligand NLX C 3



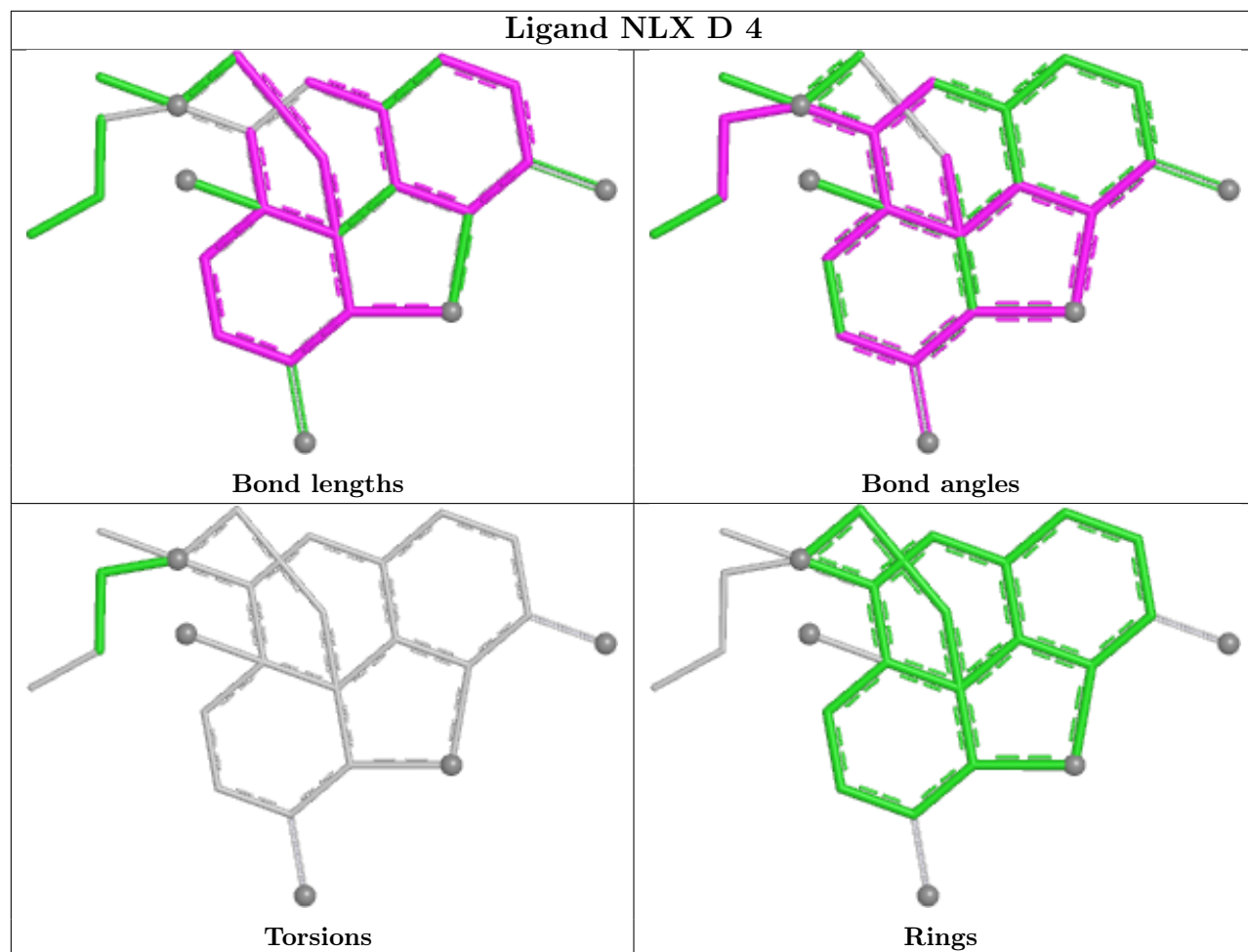
Ligand NLX L 6



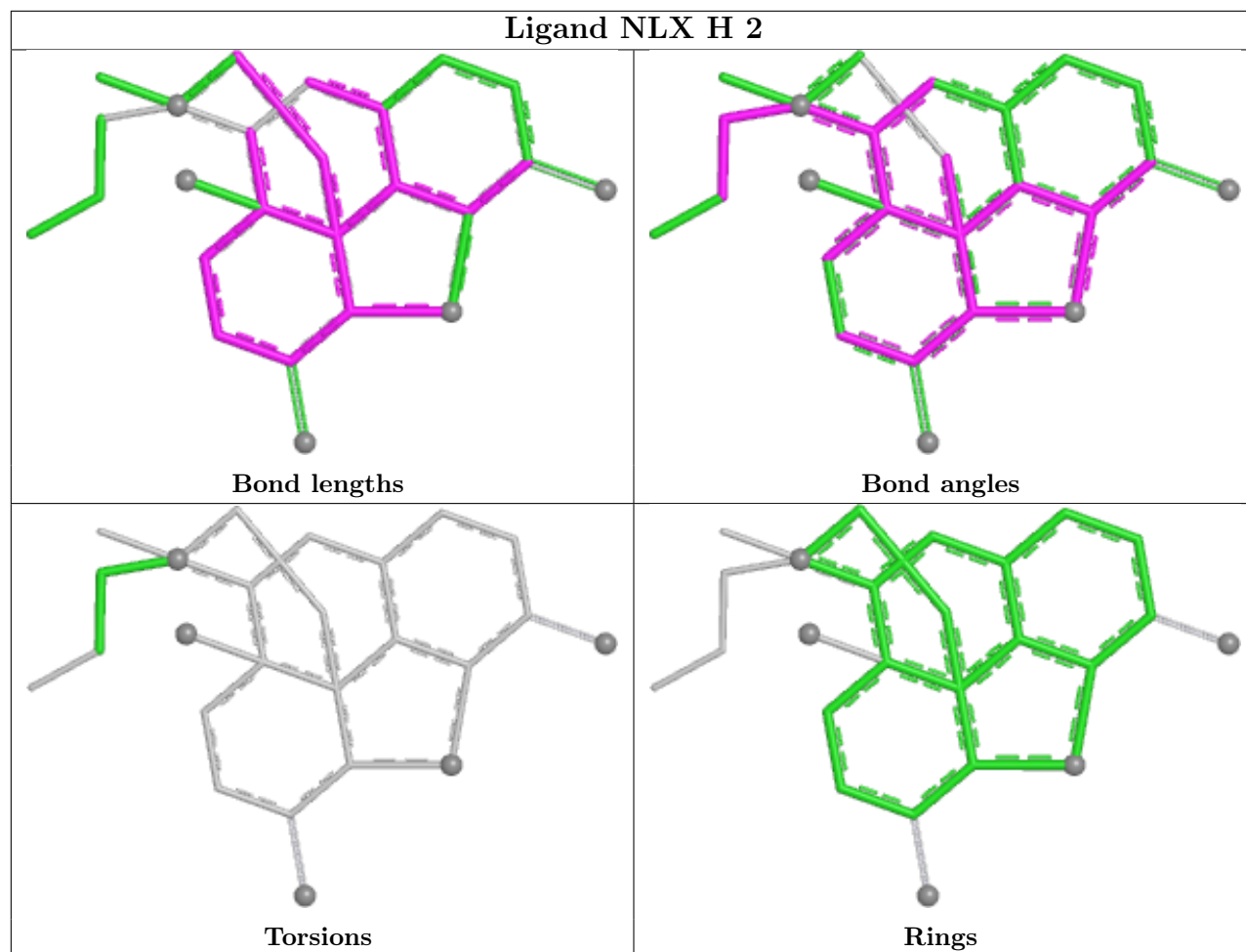
Ligand NLX K 5



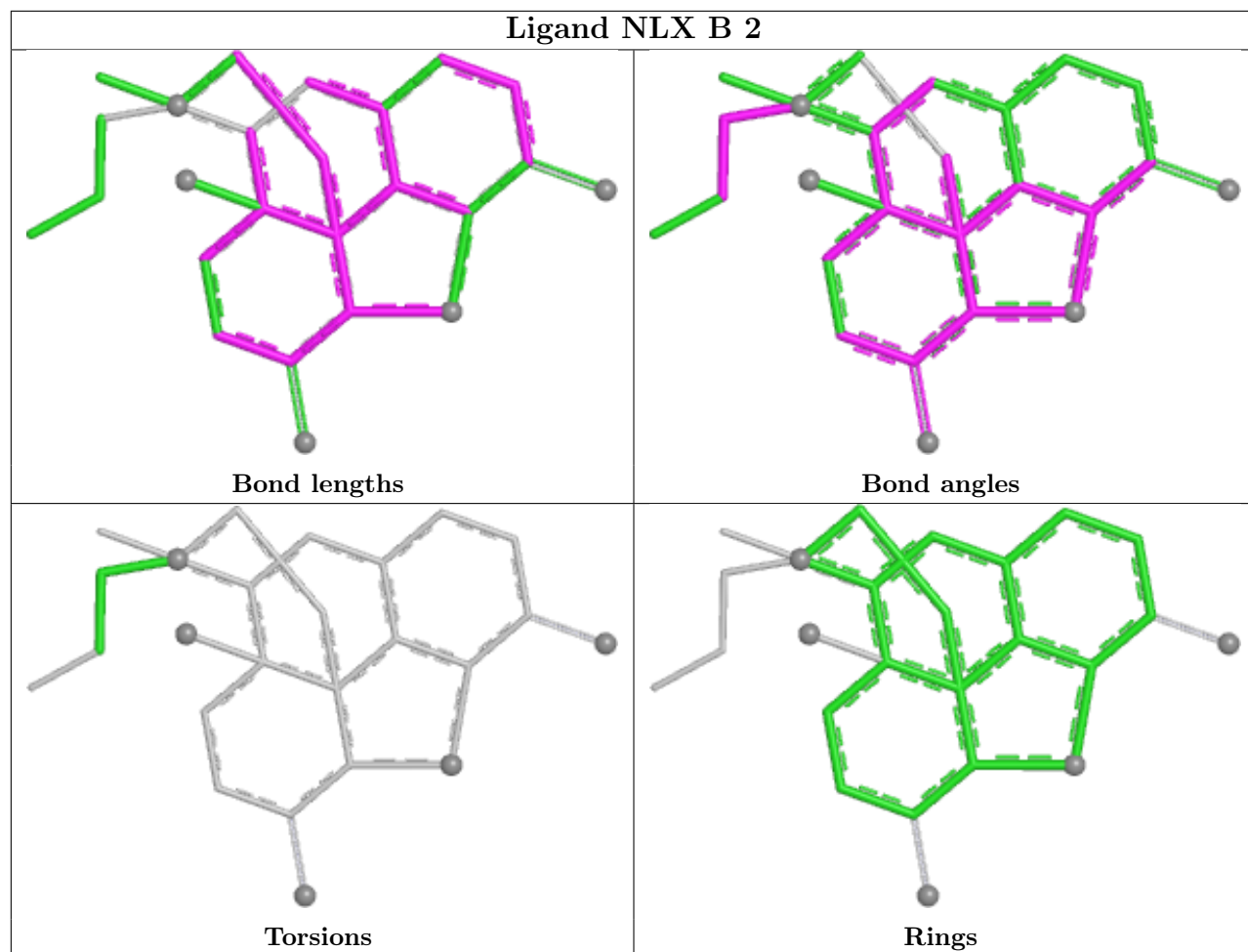
Ligand NLX D 4

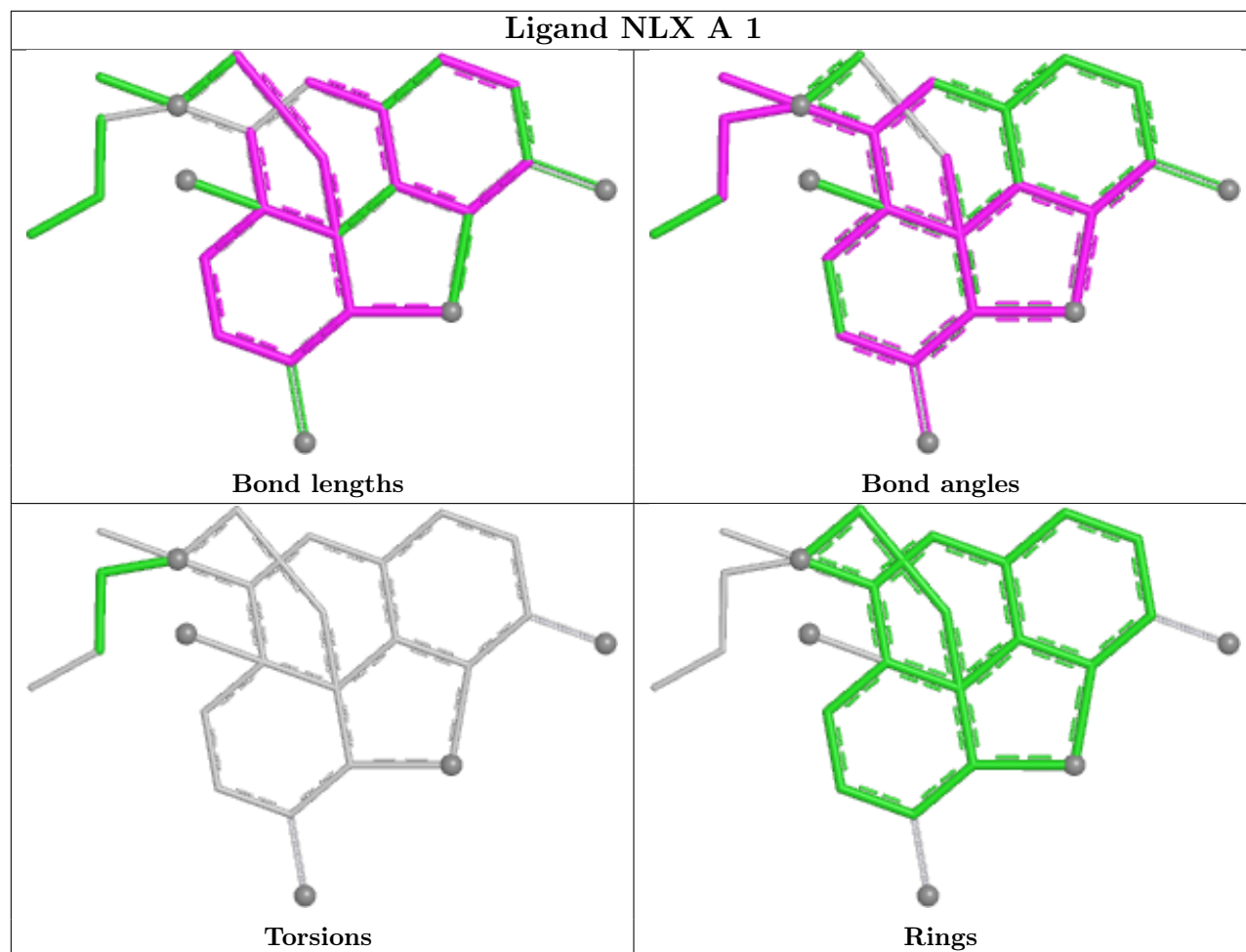


Ligand NLX H 2



Ligand NLX B 2





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.