



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:57 AM UTC

PDB ID : 1MX9 / pdb_00001mx9
Title : Crystal Structure of Human Liver Carboxylesterase in complexed with naloxone 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.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

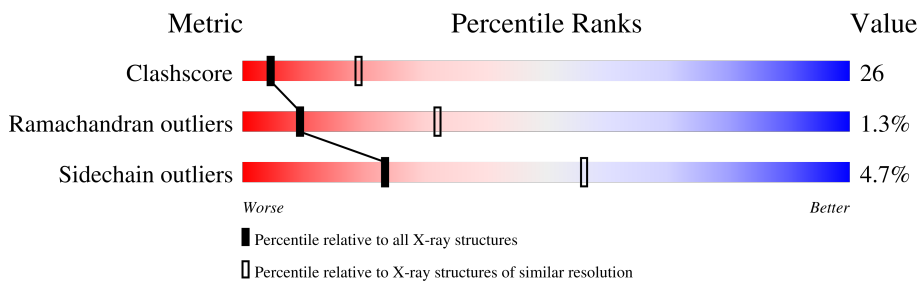
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 [i](#)

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

There are 12 discrepancies between the modelled and reference sequences:

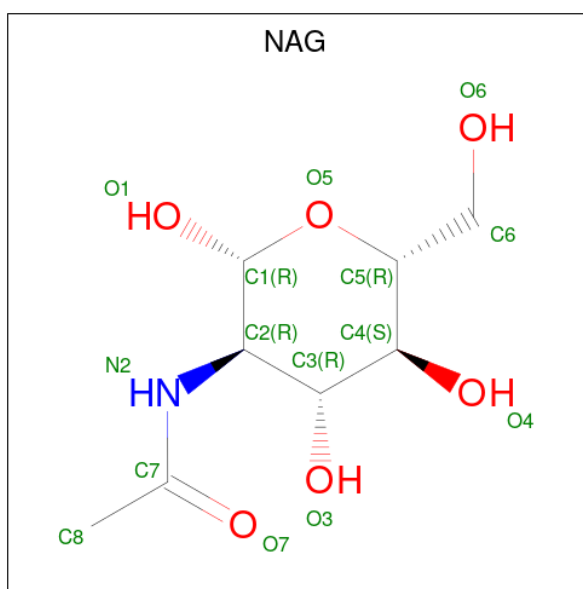
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P23141
B	?	-	GLN	deletion	UNP P23141
C	?	-	GLN	deletion	UNP P23141
D	?	-	GLN	deletion	UNP P23141
E	?	-	GLN	deletion	UNP P23141

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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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



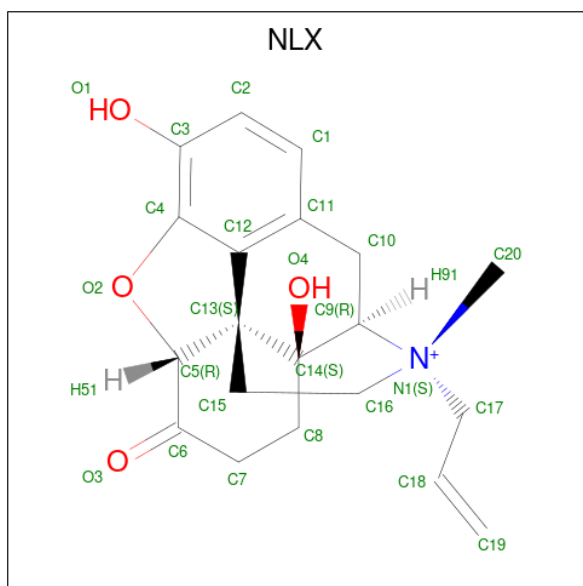
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

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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 (CCD ID: NLX) (formula: C₂₀H₂₄NO₄).



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		

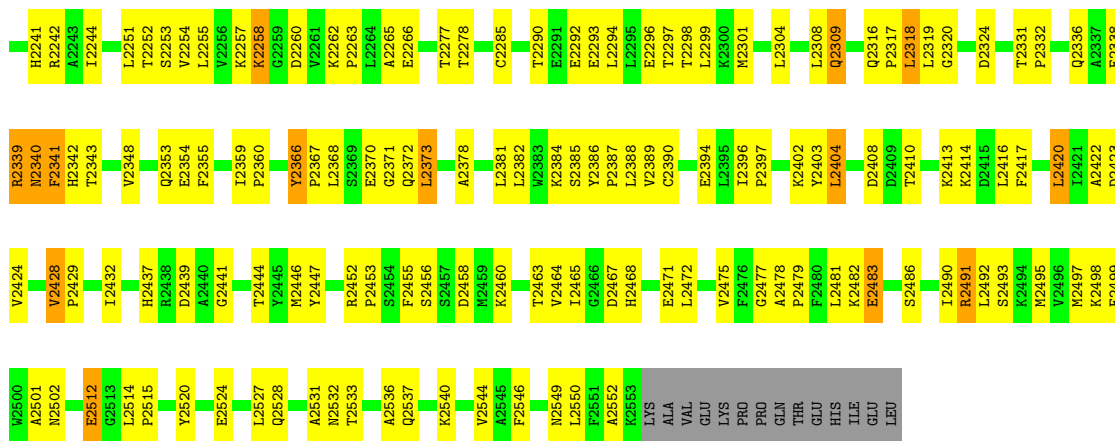
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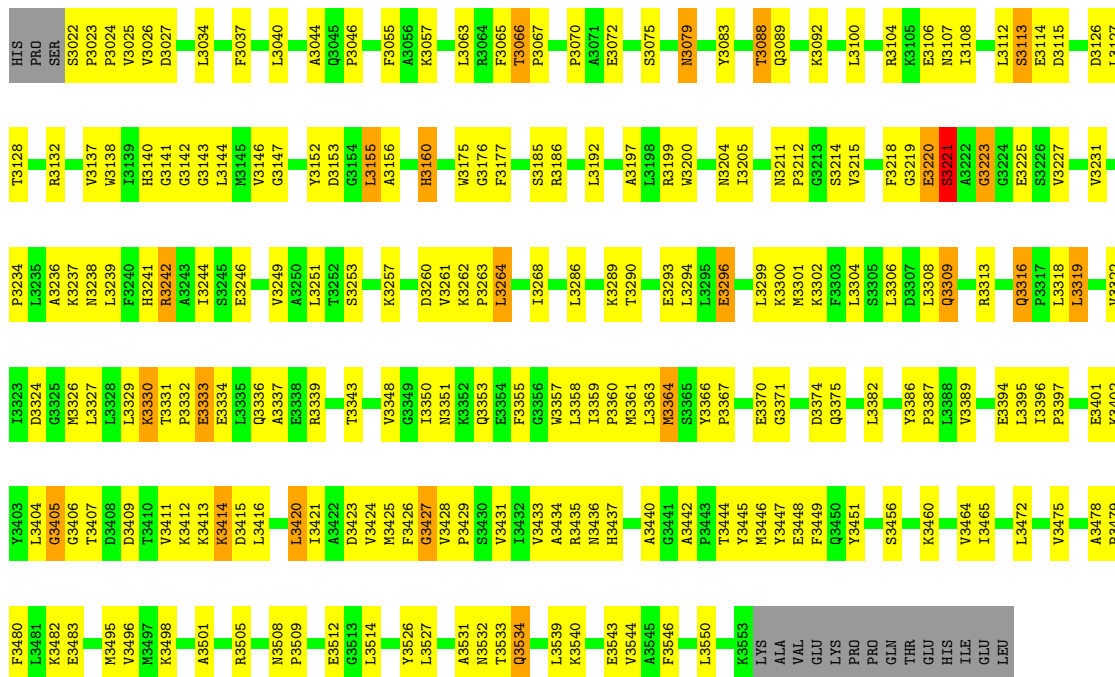
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			25	20	1	4		
3	G	1	Total	C	N	O	0	0
			25	20	1	4		
3	H	1	Total	C	N	O	0	0
			25	20	1	4		
3	I	1	Total	C	N	O	0	0
			25	20	1	4		
3	J	1	Total	C	N	O	0	0
			25	20	1	4		
3	K	1	Total	C	N	O	0	0
			25	20	1	4		
3	L	1	Total	C	N	O	0	0
			25	20	1	4		

- Molecule 4 is water.

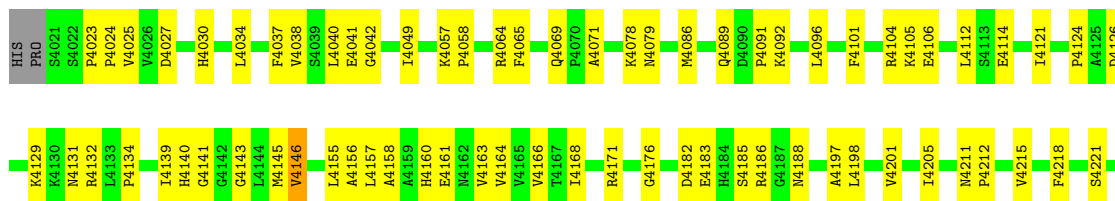
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	120	Total	O	0	0
			120	120		
4	C	98	Total	O	0	0
			98	98		
4	D	119	Total	O	0	0
			119	119		
4	E	112	Total	O	0	0
			112	112		
4	F	91	Total	O	0	0
			91	91		
4	G	69	Total	O	0	0
			69	69		
4	H	95	Total	O	0	0
			95	95		
4	I	80	Total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

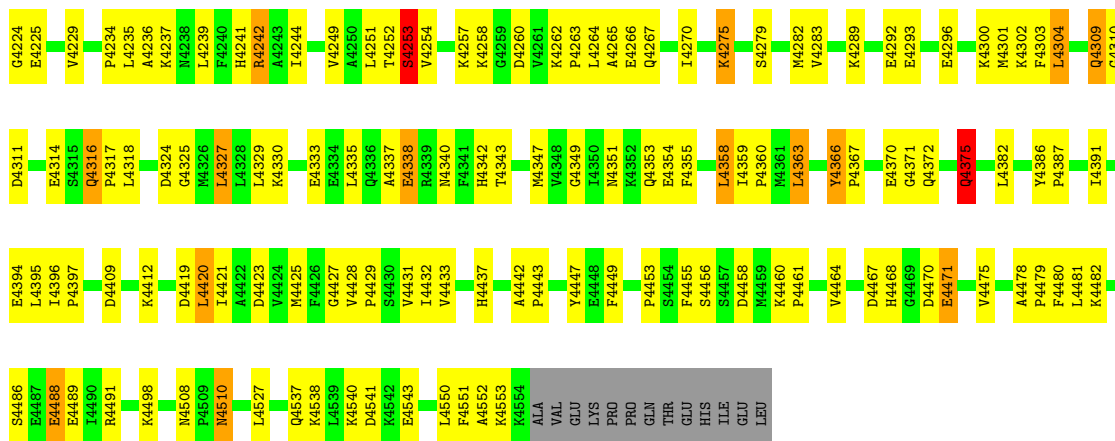


• Molecule 1: liver Carboxylesterase I

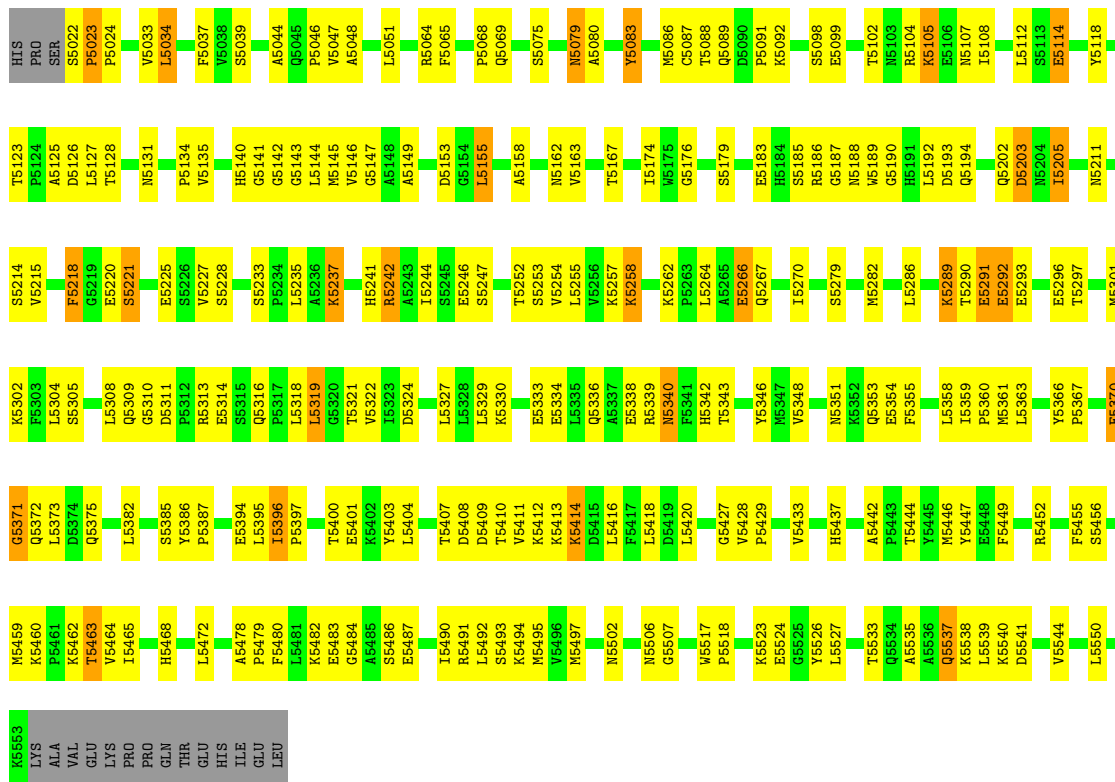


• Molecule 1: liver Carboxylesterase I

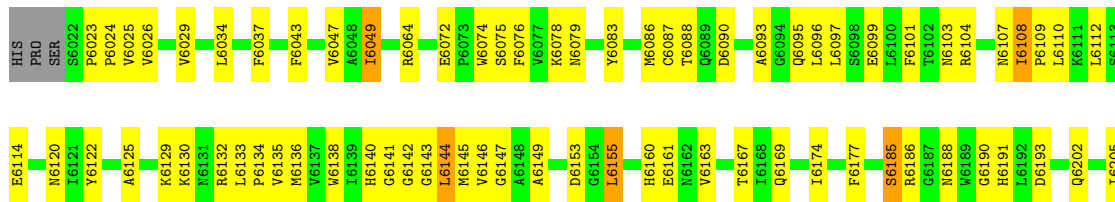


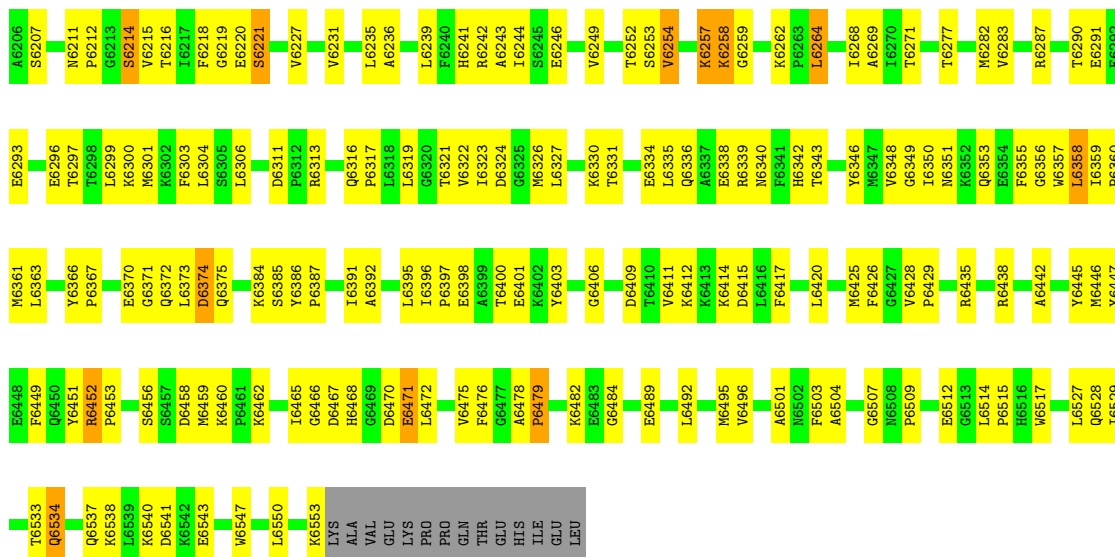


• Molecule 1: liver Carboxylesterase I

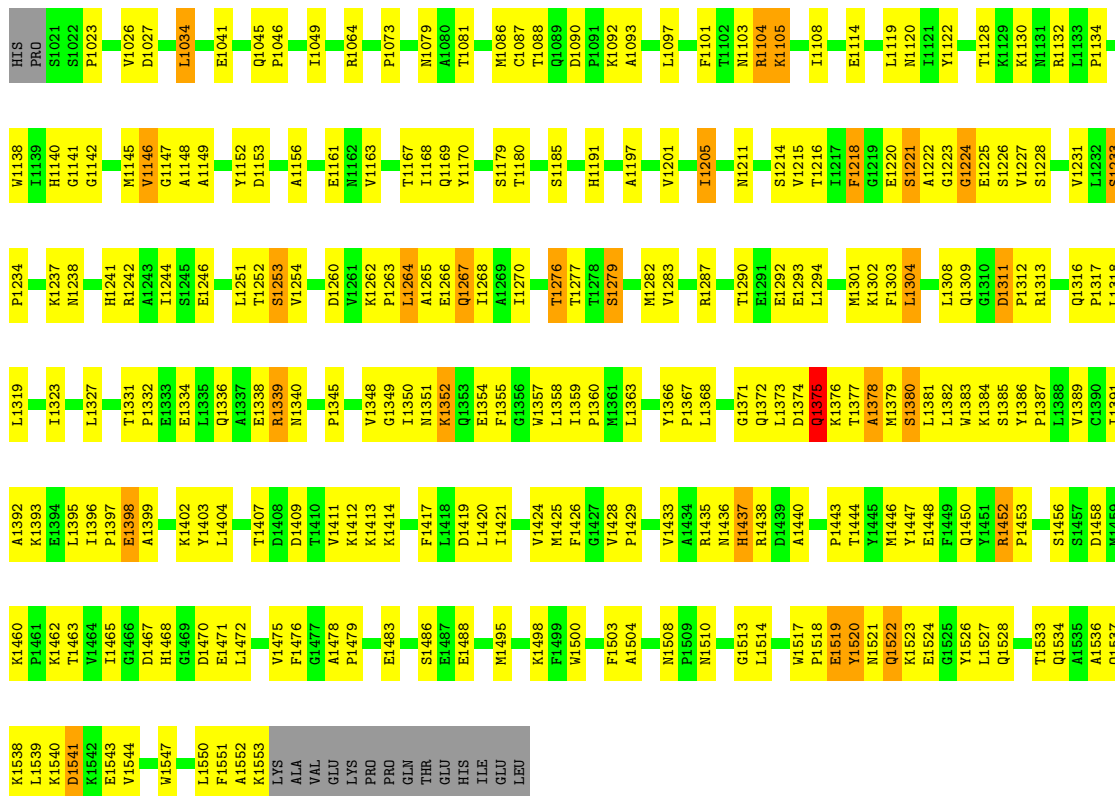


• Molecule 1: liver Carboxylesterase I





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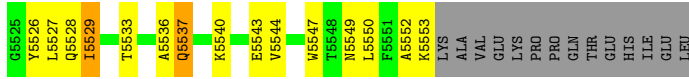


HIS	PRD	SER	S2113	E2114	L2119	L2120	L2121	L2122	L2123	D2126	L2127	L2128	K2129	G2036	K2037	L2040	E2041	A2048	K2057	G2061	R2064	E2072	T2073	W2074	K2078	N2079	T2081	S2082	Y2083	M2086	C2087	D2090	P2091	K2092	A2093	L2097	F2101	F2102	N2103	R2104	K2105	E2106	N2107	L2108	K2111	L2112				
L2299	K2300	M2301	F2302	F2303	L2304	S2305	L2306	Q2309	G2310	D2311	P2312	E2313	E2314	S2315	L2316	Q2317	L2318	L2319	D2324	L2327	K2330	E2334	E2338	R2339	R2340	F2341	T2342	T2343	P2344	P2345	Y2346	M2347	P2348	G2349	I2350	N2351	K2352	Q2353	E2354	F2355	L2358	L2359	P2360	M2361	L2363	P2366	F2367	L2368	S2369	G2371
Q2372	L2373	Q2374	Q2375	K2376	L2377	W2379	L2382	S2385	Y2386	P2387	L2388	V2389	L2396	P2397	L2398	T2400	E2401	K2402	Y2403	L2404	D2409	T2410	Y2411	K2412	K2413	K2414	F2417	L2420	D2423	V2424	M2425	F2426	G2427	V2428	P2429	R2435	M2436	H2437	R2438	A2442	P2443	Y2444	P2453	S2454	S2456					
M2459	K2460	P2461	K2462	T2463	V2464	L2465	G2466	D2467	H2468	G2469	D2470	F2471	L2472	A2478	P2479	F2480	L2481	K2482	E2483	S2486	T2490	R2491	L2492	V2496	M2497	K2498	F2499	W2500	N2501	N2502	R2505	L2514	E2524	G2525	K2526	L2527	Q2528	Q2534	A2535	A2536	Q2537	K2538	L2539	K2540	E2543	V2544	A2545	W2546	P2547	
K2553	LYS	ALA	VAL	VAL	GLU	LYS	PRO	PRO	GLN	THR	GLU	HIS	ILE	GLU	LEU																																			

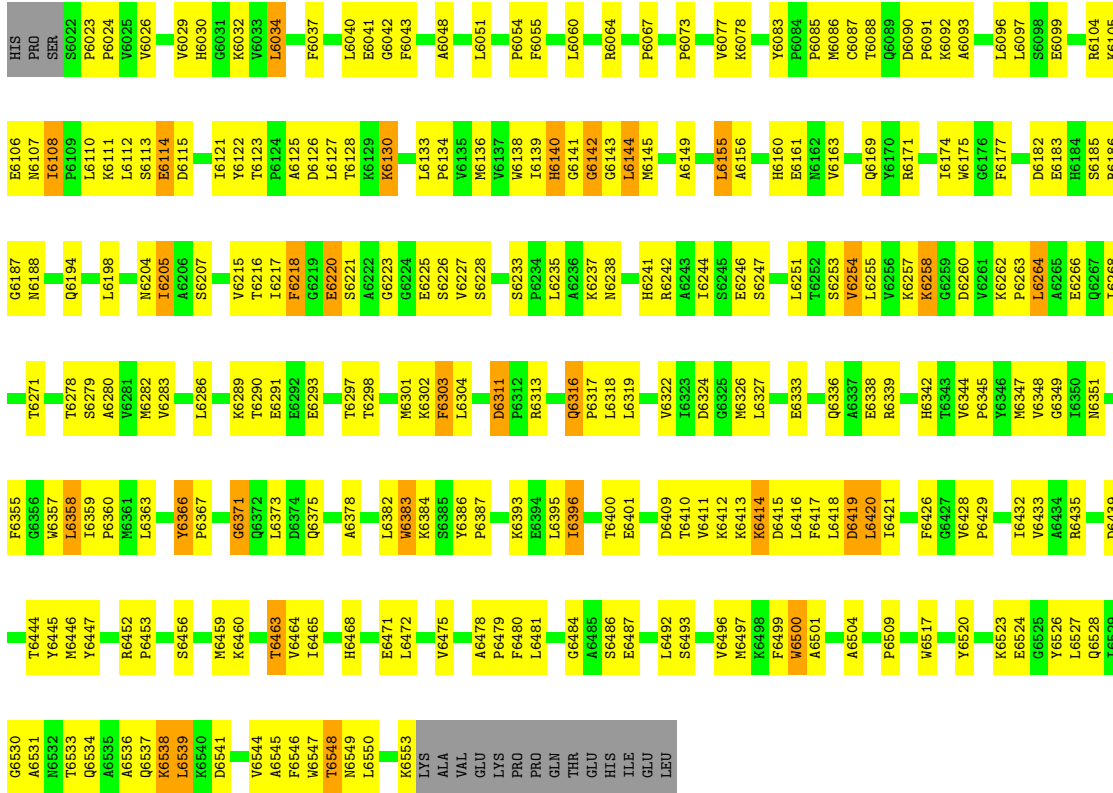
• Molecule 1: liver Carboxylesterase I



HIS	PRD	SER	P3124	A3125	D3126	S3022	P3023	P3024	V3025	V3026	D3027	V3028	V3029	V3033	L3034	F3037	V3038	S3039	F3043	A3044	Q3045	P3046	F3050	K3057	L3063	K3064	K3065	E3072	N3079	C3087	T3088	Q3089	D3090	P3091	K3092	A3093	K3094	Q3095	L3096	N3103	R3104	K3105	E3106	N3107	L3108	L3112	S3113	L3119	T3123										
V3281	H3284	C3285	L3286	R3287	Q3288	K3289	T3290	E3293	L3294	A3295	E3296	T3297	T3298	L3299	K3300	K3301	M3301	K3302	F3303	L3304	Q3309	Q3316	P3317	L3318	L3319	L3320	L3321	P3324	L3325	A3326	K3327	N3328	L3329	F3329	H3329	R3342	A3343	L3344	G3345	H3360	R3361	R3362	V3363	V3364	I3368	G3373	F3377	P3381	T3380	S3185	H3191	V3195	R3199	K3200	N3204	I3205	A3206	G3210	N3211
V3215	T3216	F3218	G3219	E3220	S3221	A3222	G3224	E3225	S3226	V3227	S3228	V3229	L3230	V3231	P3234	L3235	A3236	K3237	N3238	F3240	H3241	R3242	A3243	L3244	G3245	S3246	V3249	A3250	L3251	T3252	S3253	V3254	L3256	V3256	K3257	K3258	K3262	P3263	L3264	A3265	E3266	Q3267	L3268	A3269	L3270	A3272	K3275	F3276	T3277	T3278									
V3281	H3284	C3285	L3286	R3287	Q3288	K3289	T3290	E3293	L3294	A3295	E3296	T3297	T3298	L3299	K3300	K3301	M3301	K3302	F3303	L3304	Q3309	Q3316	P3317	L3318	L3319	L3320	V3231	P3324	L3325	A3326	K3327	N3328	L3329	F3329	H3329	R3342	A3343	L3344	G3345	H3360	R3361	R3362	V3363	V3364	I3368	G3373	F3377	P3381	T3380	S3185	H3191	V3195	R3199	K3200	N3204	I3205	A3206	G3210	N3211
N3351	K3352	E3353	E3354	F3355	G3356	K3357	L3358	L3359	P3360	L3363	A3364	S3365	P3367	L3368	S3369	E3370	G3371	Q3372	L3373	D3374	L3381	L3382	W3383	K3384	S3385	Y3386	P3387	L3388	L3389	C3390	L3391	G3392	K3393	E3394	L3395	L3396	P3397	E3398	A3399	T3400	L3404	T3407	T3410	V3411	K3412	T3413	K3414	K3415	D3416	L3416	L3420	L3421	A3422						
V3423	V3424	M3425	F3426	N3510	G3511	G3512	G3513	L3514	W3515	W3517	A3526	Q3534	A3535	K3538	L3539	K3540	D3541	K3542	P3543	S3547	T3548	N3549	L3550	K3553	LYS	ALA	VAL	GLU	LYS	PRO	PRO	GLN	THR	GLU	HIS	ILE	GLU	LEU																					



● Molecule 1: liver Carboxylesterase I



4 Data and refinement statistics

Xtrriage (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.	Xtrriage
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: NAG, NLX

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	0.46	0/4236	0.98	15/5754 (0.3%)
1	B	0.51	0/4236	1.02	17/5754 (0.3%)
1	C	0.52	1/4230 (0.0%)	0.99	15/5746 (0.3%)
1	D	0.50	0/4241	0.97	10/5761 (0.2%)
1	E	0.49	0/4230	0.98	16/5746 (0.3%)
1	F	0.47	0/4230	1.00	17/5746 (0.3%)
1	G	0.45	0/4236	0.94	11/5754 (0.2%)
1	H	0.48	0/4230	1.03	19/5746 (0.3%)
1	I	0.44	0/4230	0.95	11/5746 (0.2%)
1	J	0.49	0/4236	0.96	7/5754 (0.1%)
1	K	0.44	0/4230	0.96	13/5746 (0.2%)
1	L	0.45	0/4230	0.97	15/5746 (0.3%)
All	All	0.47	1/50795 (0.0%)	0.98	166/68999 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3364	MET	SD-CE	7.77	1.99	1.79

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	6140	HIS	N-CA-C	11.19	124.53	111.11
1	B	2075	SER	N-CA-C	11.15	125.41	111.69
1	B	2339	ARG	N-CA-C	9.53	125.50	111.02
1	E	5075	SER	N-CA-C	8.86	124.50	112.90
1	A	1075	SER	N-CA-C	8.24	121.83	111.69

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	244	0
1	B	4130	0	4132	195	0
1	C	4124	0	4127	186	0
1	D	4135	0	4134	174	0
1	E	4124	0	4127	212	0
1	F	4124	0	4127	208	0
1	G	4130	0	4132	254	0
1	H	4124	0	4127	204	0
1	I	4124	0	4127	241	0
1	J	4130	0	4134	226	0
1	K	4124	0	4127	239	0
1	L	4124	0	4127	260	0
2	A	28	0	26	3	0
2	B	14	0	13	5	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	14	0	13	1	0
2	L	14	0	13	0	0
3	A	25	0	23	21	0
3	B	25	0	23	21	0
3	C	25	0	19	28	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	31	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	9	0
4	G	69	0	0	9	0
4	H	95	0	0	10	0
4	I	80	0	0	10	0
4	J	110	0	0	9	0
4	K	73	0	0	11	0
4	L	75	0	0	16	0
All	All	51134	0	49998	2599	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 26.

The worst 5 of 2599 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	26
1	B	530/548 (97%)	476 (90%)	48 (9%)	6 (1%)	11	36
1	C	529/548 (96%)	489 (92%)	33 (6%)	7 (1%)	9	32
1	D	531/548 (97%)	491 (92%)	36 (7%)	4 (1%)	16	44
1	E	529/548 (96%)	482 (91%)	40 (8%)	7 (1%)	9	32
1	F	529/548 (96%)	477 (90%)	44 (8%)	8 (2%)	8	28
1	G	530/548 (97%)	467 (88%)	55 (10%)	8 (2%)	8	28
1	H	529/548 (96%)	470 (89%)	52 (10%)	7 (1%)	9	32
1	I	529/548 (96%)	466 (88%)	56 (11%)	7 (1%)	9	32
1	J	530/548 (97%)	484 (91%)	40 (8%)	6 (1%)	11	36
1	K	529/548 (96%)	475 (90%)	48 (9%)	6 (1%)	11	36
1	L	529/548 (96%)	467 (88%)	53 (10%)	9 (2%)	7	26
All	All	6354/6576 (97%)	5724 (90%)	546 (9%)	84 (1%)	9	32

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	71
1	B	448/463 (97%)	432 (96%)	16 (4%)	31	65
1	C	447/463 (96%)	422 (94%)	25 (6%)	19	50
1	D	448/463 (97%)	425 (95%)	23 (5%)	21	53
1	E	447/463 (96%)	426 (95%)	21 (5%)	23	56
1	F	447/463 (96%)	432 (97%)	15 (3%)	32	66
1	G	448/463 (97%)	419 (94%)	29 (6%)	15	44
1	H	447/463 (96%)	429 (96%)	18 (4%)	28	62
1	I	447/463 (96%)	422 (94%)	25 (6%)	19	50
1	J	448/463 (97%)	423 (94%)	25 (6%)	19	50
1	K	447/463 (96%)	423 (95%)	24 (5%)	20	51
1	L	447/463 (96%)	431 (96%)	16 (4%)	31	65
All	All	5369/5556 (97%)	5119 (95%)	250 (5%)	23	56

5 of 250 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	1104	ARG
1	K	5292	GLU
1	H	2111	LYS
1	K	5240	PHE
1	L	6130	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 199 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	1309	GLN
1	I	3267	GLN
1	G	1375	GLN
1	H	2316	GLN
1	I	3534	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	379	-	14,14,15	0.48	0	17,19,21	0.76	0
2	NAG	E	579	-	14,14,15	0.52	0	17,19,21	0.80	1 (5%)
3	NLX	K	5	-	26,29,29	3.23	14 (53%)	44,49,49	2.05	12 (27%)
3	NLX	G	1	-	26,29,29	3.47	15 (57%)	44,49,49	2.19	12 (27%)
2	NAG	J	479	-	14,14,15	0.56	0	17,19,21	0.67	0
3	NLX	A	1	-	26,29,29	3.76	15 (57%)	44,49,49	2.14	15 (34%)
3	NLX	L	6	-	26,29,29	3.42	16 (61%)	44,49,49	2.15	13 (29%)
3	NLX	D	4	-	26,29,29	3.37	16 (61%)	44,49,49	2.23	13 (29%)
2	NAG	K	579	-	14,14,15	0.53	0	17,19,21	0.78	1 (5%)
3	NLX	I	3	-	26,29,29	3.22	17 (65%)	44,49,49	2.33	14 (31%)
2	NAG	D	479	-	14,14,15	0.45	0	17,19,21	0.64	0
3	NLX	F	6	-	26,29,29	3.44	18 (69%)	44,49,49	4.85	23 (52%)
3	NLX	J	4	-	26,29,29	3.49	14 (53%)	44,49,49	1.98	12 (27%)
2	NAG	G	179	-	14,14,15	0.57	0	17,19,21	0.60	0
2	NAG	F	679	-	14,14,15	0.51	0	17,19,21	0.79	1 (5%)
2	NAG	I	379	-	14,14,15	0.47	0	17,19,21	0.82	1 (5%)
2	NAG	H	279	-	14,14,15	0.49	0	17,19,21	0.68	0
3	NLX	E	5	-	26,29,29	3.13	16 (61%)	44,49,49	2.01	13 (29%)
3	NLX	C	3	-	26,29,29	4.49	17 (65%)	44,49,49	4.63	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	179	-	14,14,15	0.66	0	17,19,21	0.68	0
2	NAG	B	279	-	14,14,15	0.50	0	17,19,21	0.61	0
2	NAG	L	679	-	14,14,15	0.62	0	17,19,21	0.67	0
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%)
2	NAG	A	180	-	14,14,15	0.61	0	17,19,21	0.68	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	NAG	C	379	-	-	2/6/23/26	0/1/1/1
2	NAG	E	579	-	-	0/6/23/26	0/1/1/1
3	NLX	K	5	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	G	1	-	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	A	1	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	L	6	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	D	4	-	1/1/6/7	0/4/62/62	0/6/5/5
2	NAG	K	579	-	-	4/6/23/26	0/1/1/1
3	NLX	I	3	-	1/1/6/7	1/4/62/62	0/6/5/5
2	NAG	D	479	-	-	2/6/23/26	0/1/1/1
3	NLX	F	6	-	1/1/6/7	2/4/62/62	0/6/5/5
3	NLX	J	4	-	1/1/6/7	0/4/62/62	0/6/5/5
2	NAG	G	179	-	-	5/6/23/26	0/1/1/1
2	NAG	F	679	-	-	3/6/23/26	0/1/1/1
2	NAG	I	379	-	-	4/6/23/26	0/1/1/1
2	NAG	H	279	-	-	4/6/23/26	0/1/1/1
3	NLX	E	5	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	C	3	-	1/1/6/7	1/4/62/62	0/6/5/5
2	NAG	A	179	-	-	4/6/23/26	0/1/1/1
2	NAG	B	279	-	-	2/6/23/26	0/1/1/1
2	NAG	L	679	-	-	2/6/23/26	0/1/1/1
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
2	NAG	A	180	-	-	2/6/23/26	0/1/1/1

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 277 short contacts:

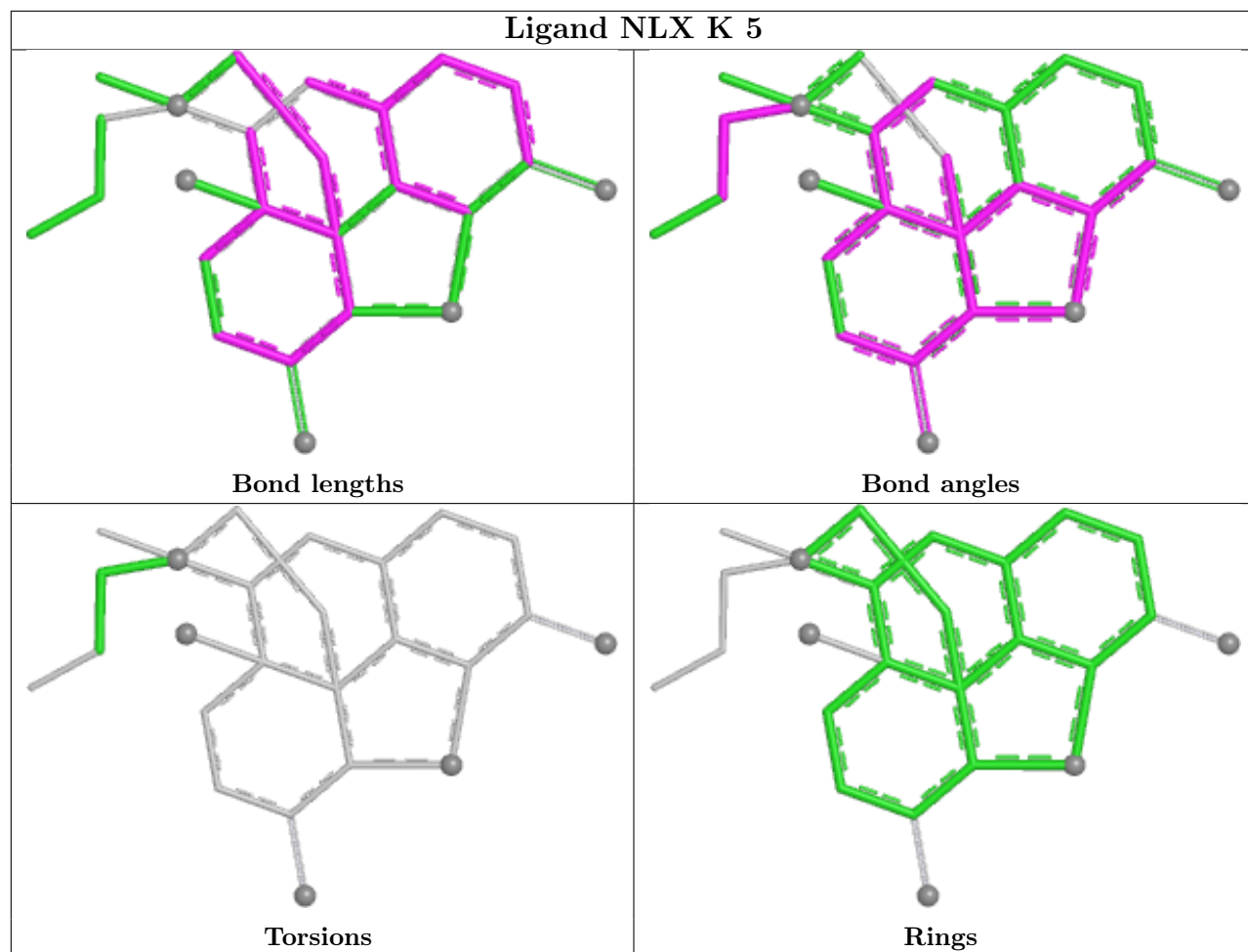
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	579	NAG	2	0
3	K	5	NLX	18	0
3	G	1	NLX	12	0
2	J	479	NAG	7	0

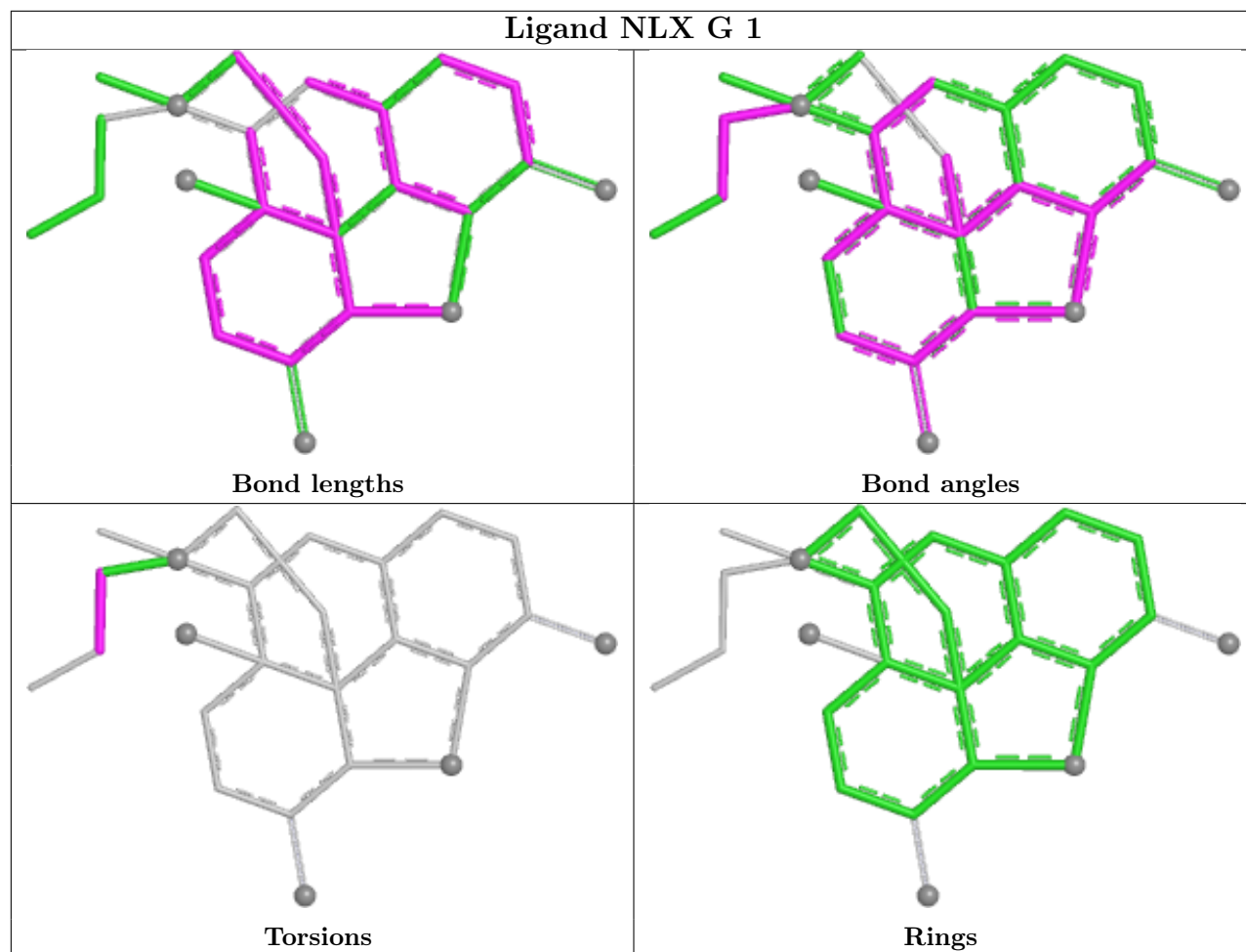
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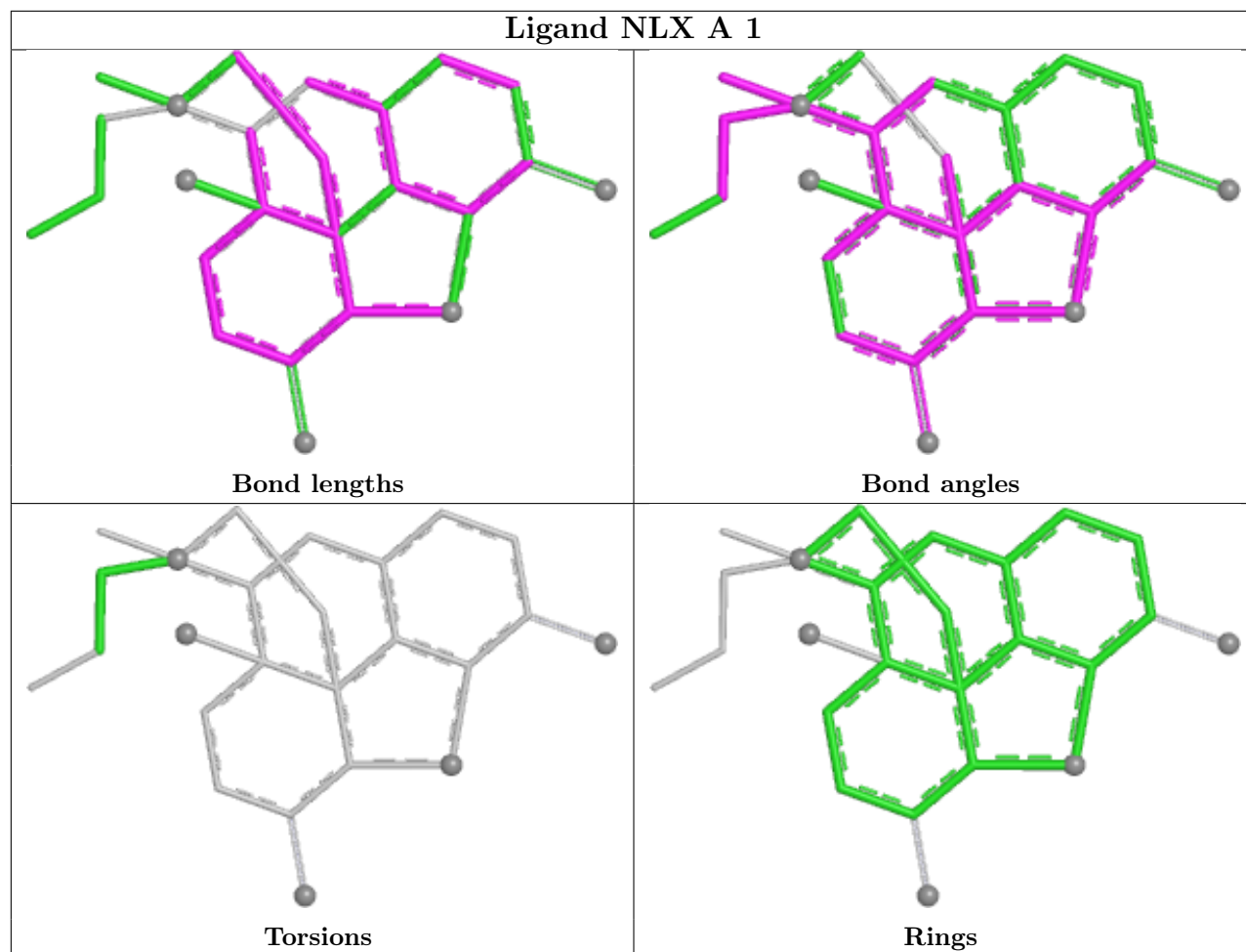
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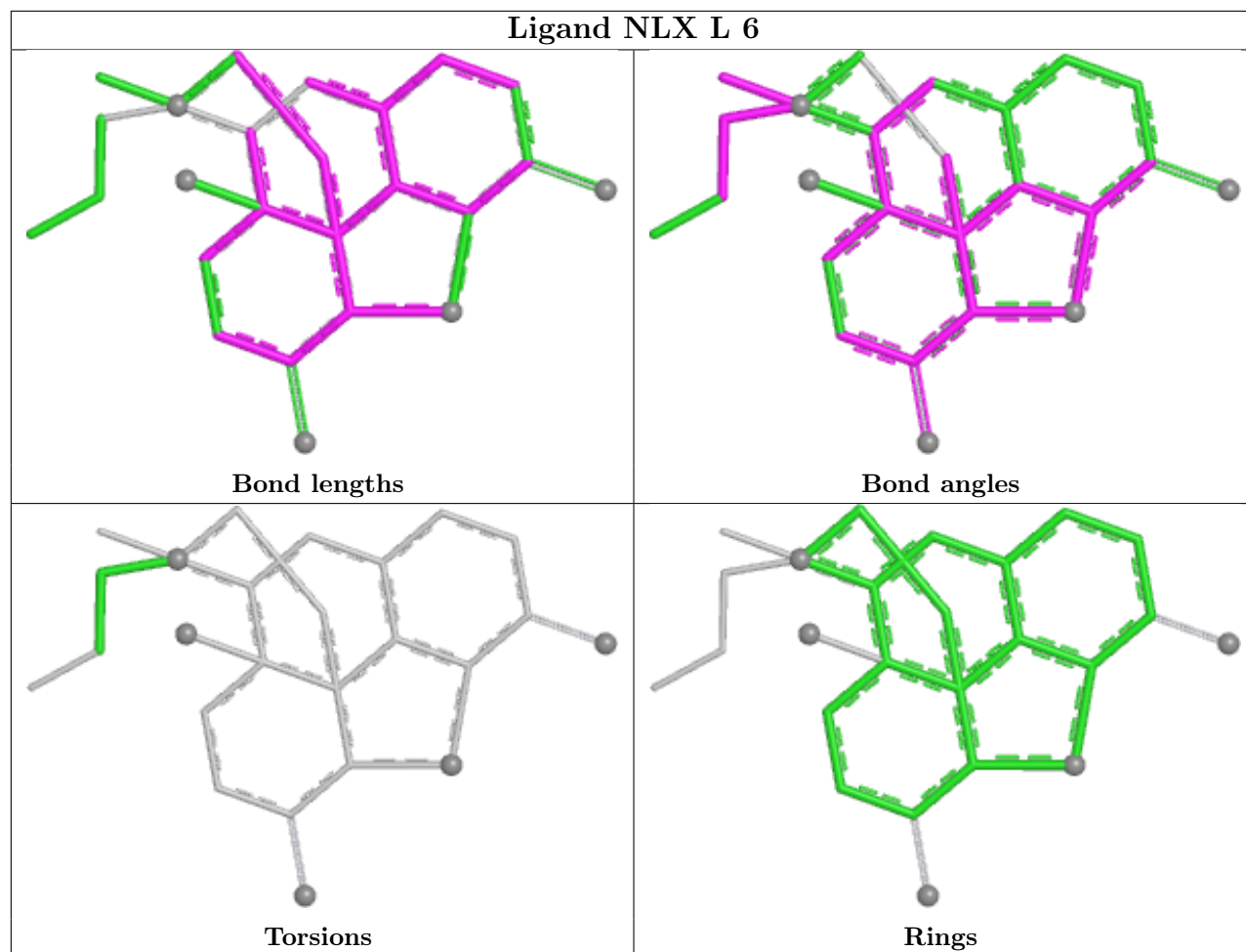
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NLX	21	0
3	L	6	NLX	23	0
3	D	4	NLX	15	0
2	K	579	NAG	1	0
3	I	3	NLX	19	0
2	D	479	NAG	4	0
3	F	6	NLX	23	0
3	J	4	NLX	20	0
2	G	179	NAG	4	0
2	I	379	NAG	1	0
2	H	279	NAG	1	0
3	E	5	NLX	18	0
3	C	3	NLX	28	0
2	A	179	NAG	3	0
2	B	279	NAG	5	0
3	H	2	NLX	31	0
3	B	2	NLX	21	0
2	A	180	NAG	1	0

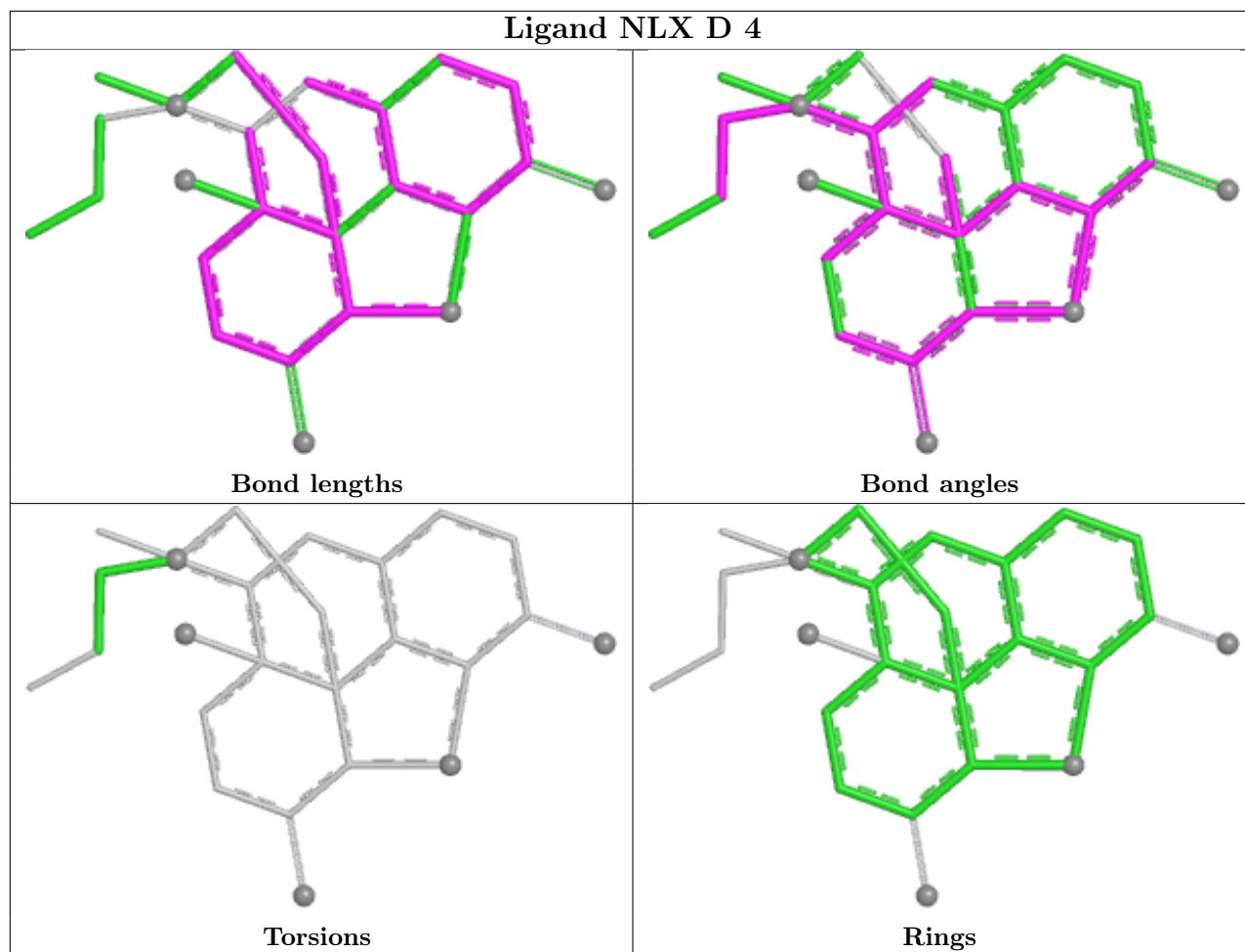
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

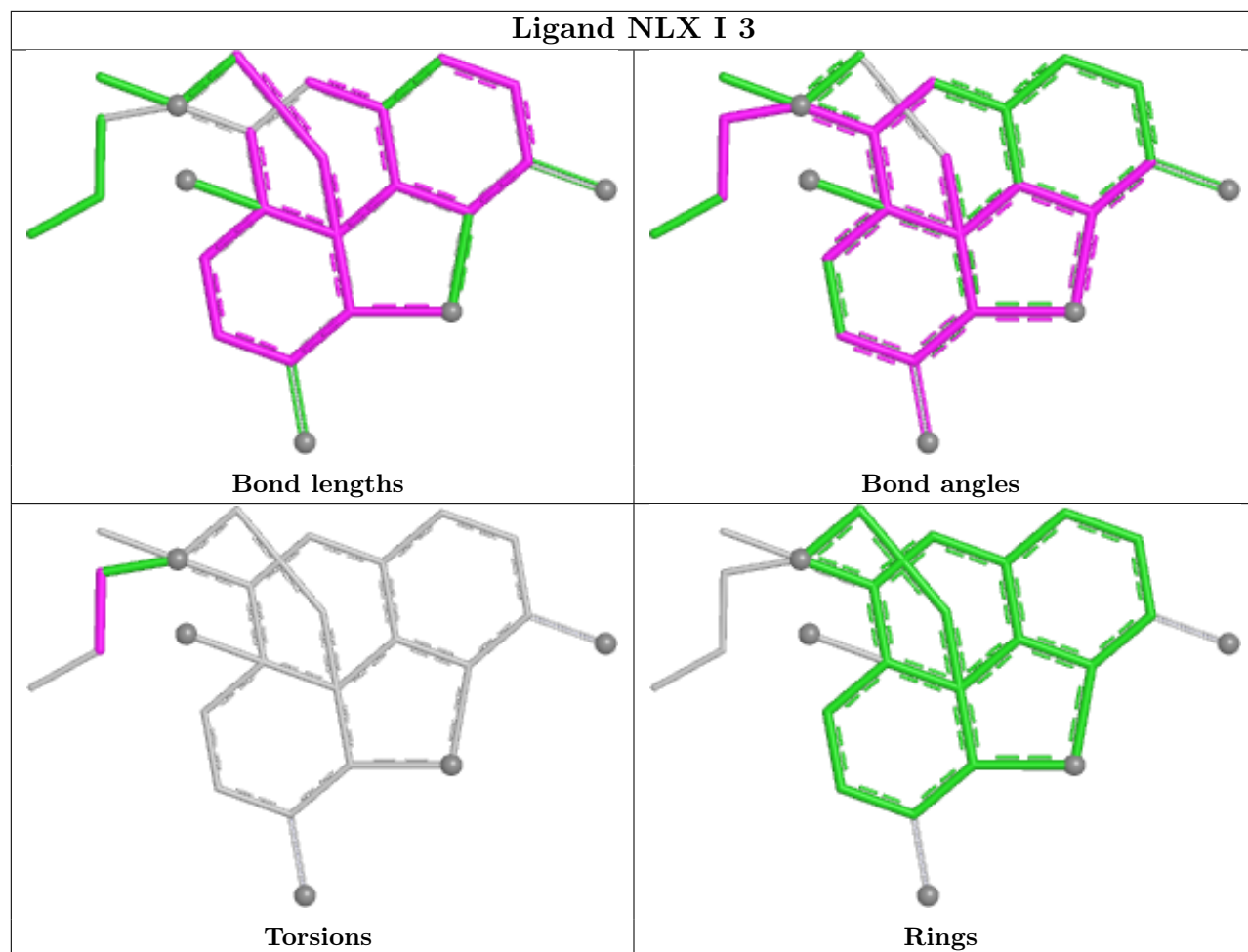


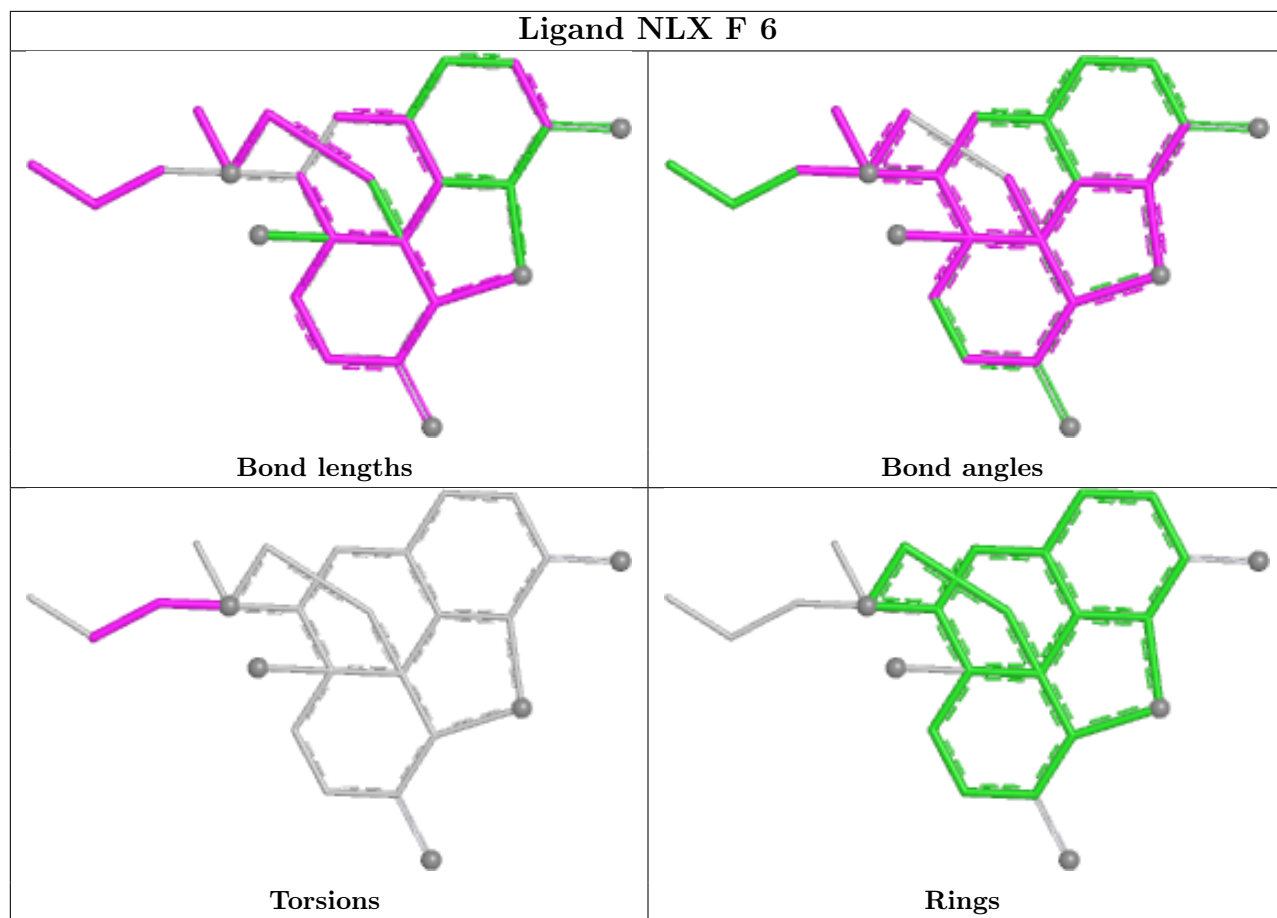


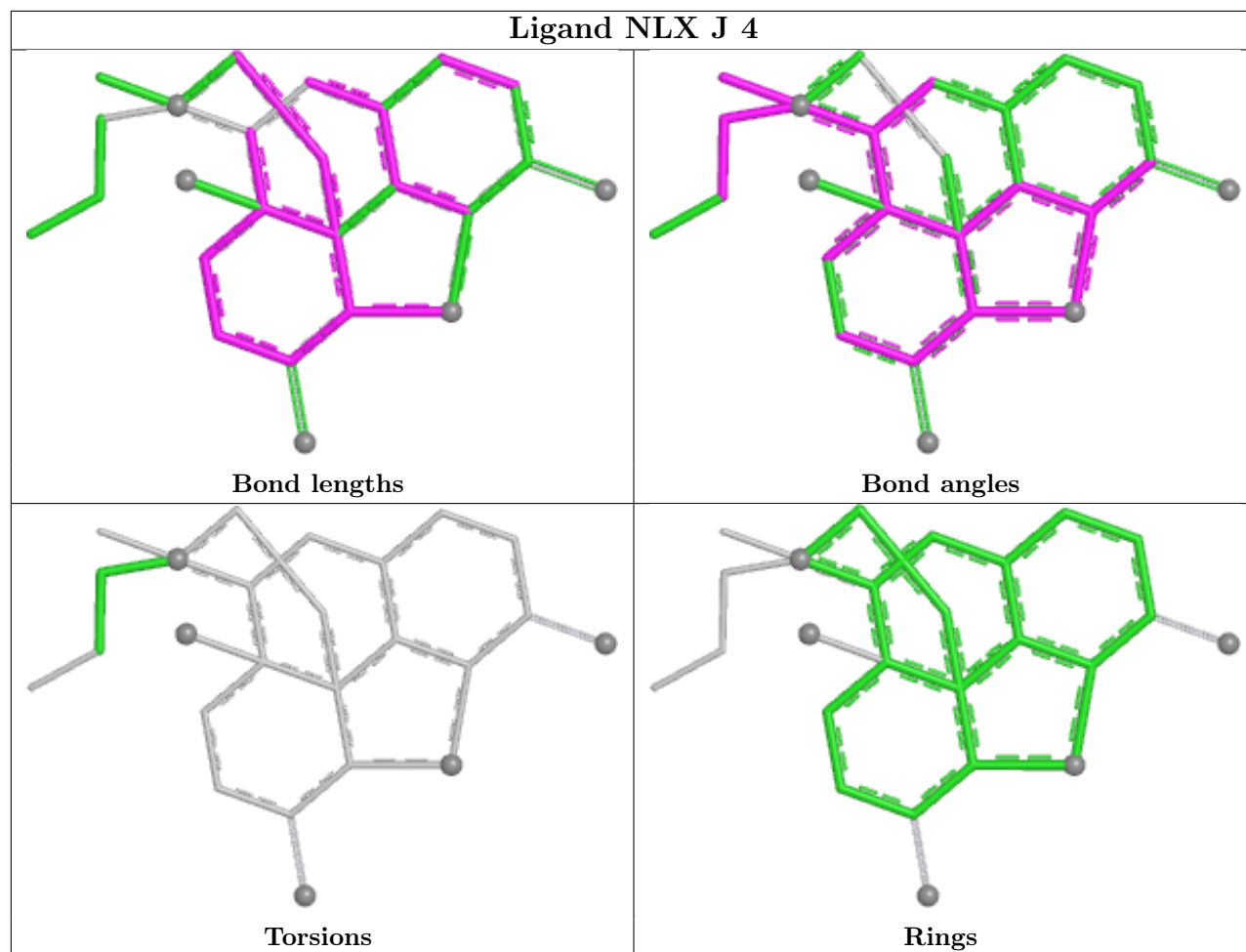


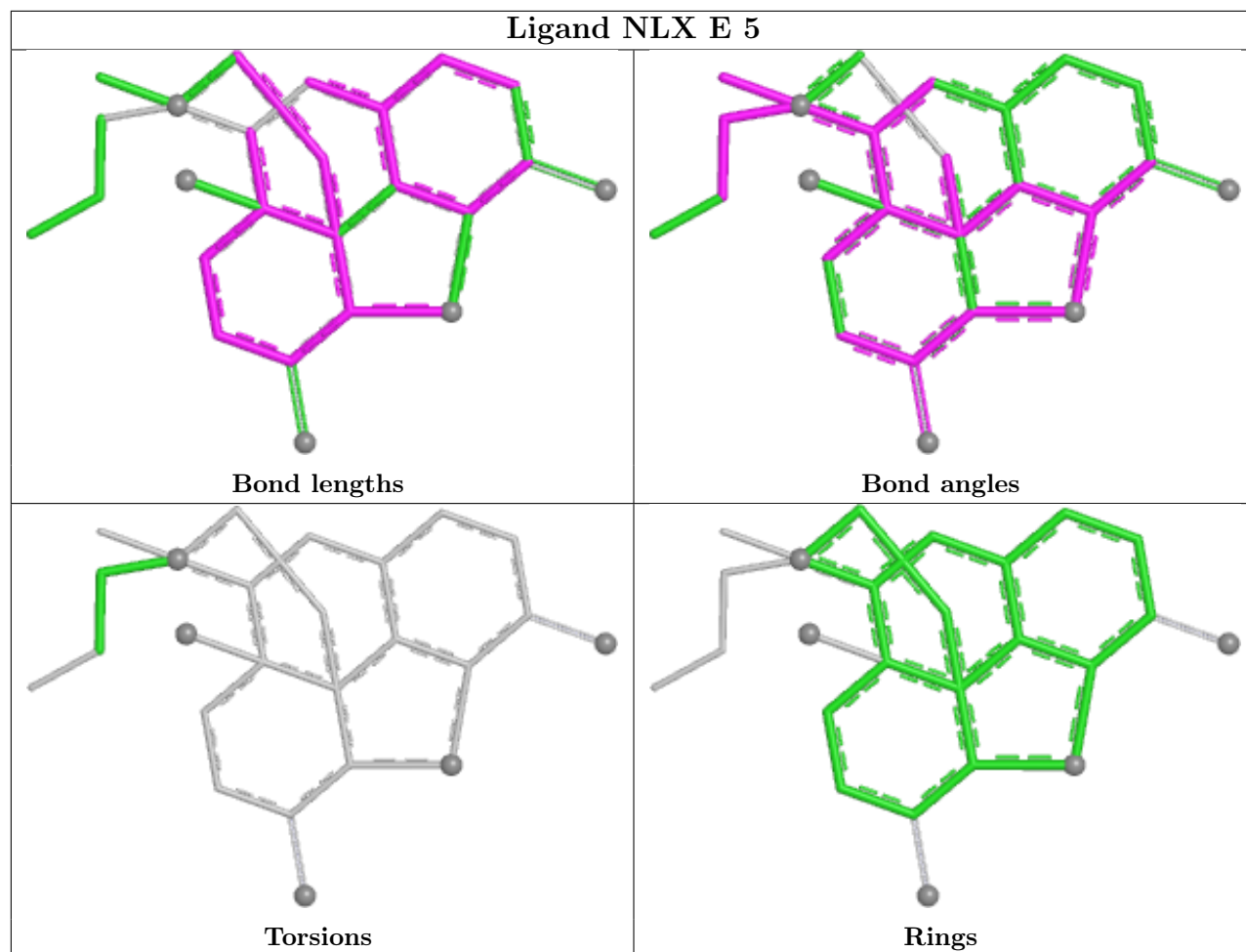


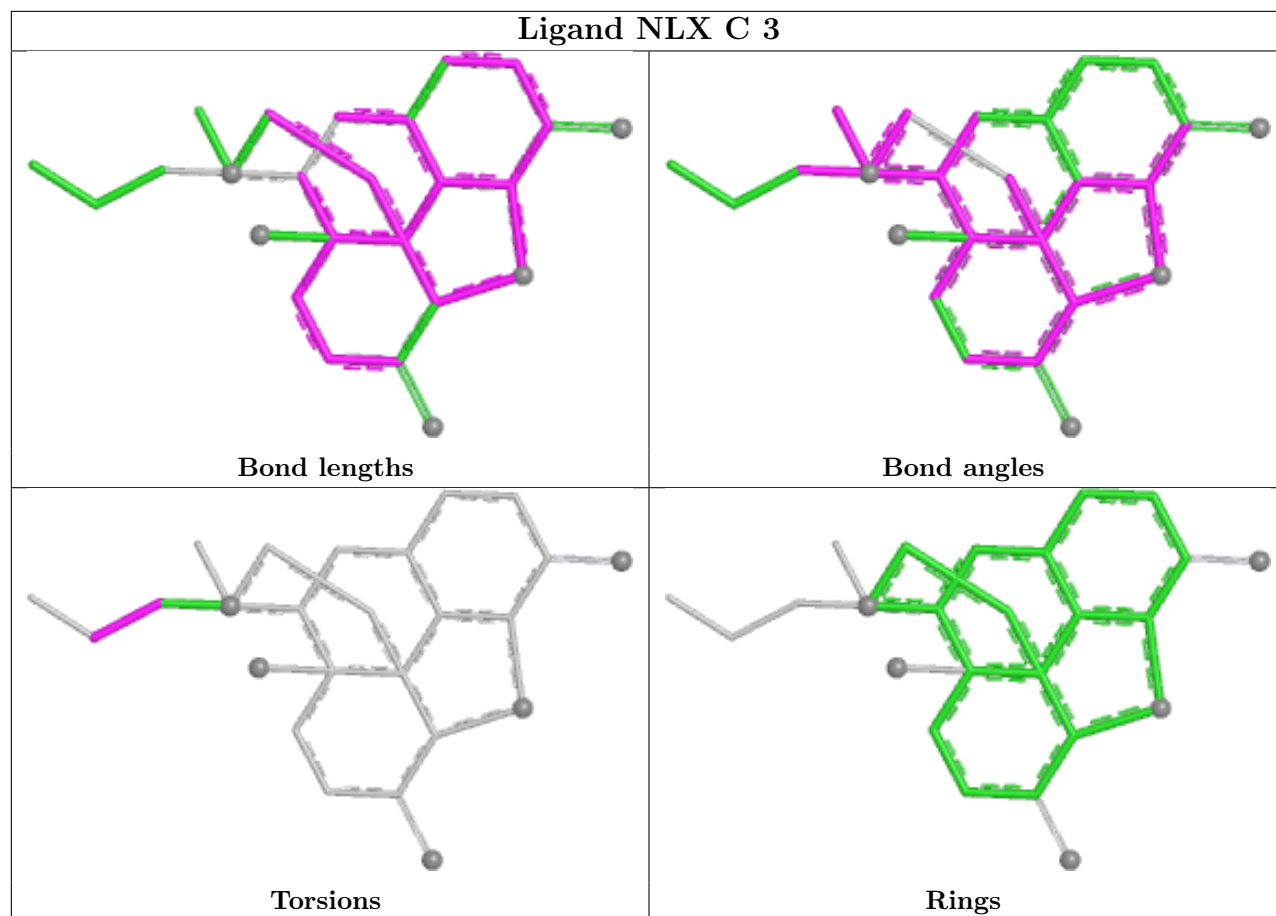


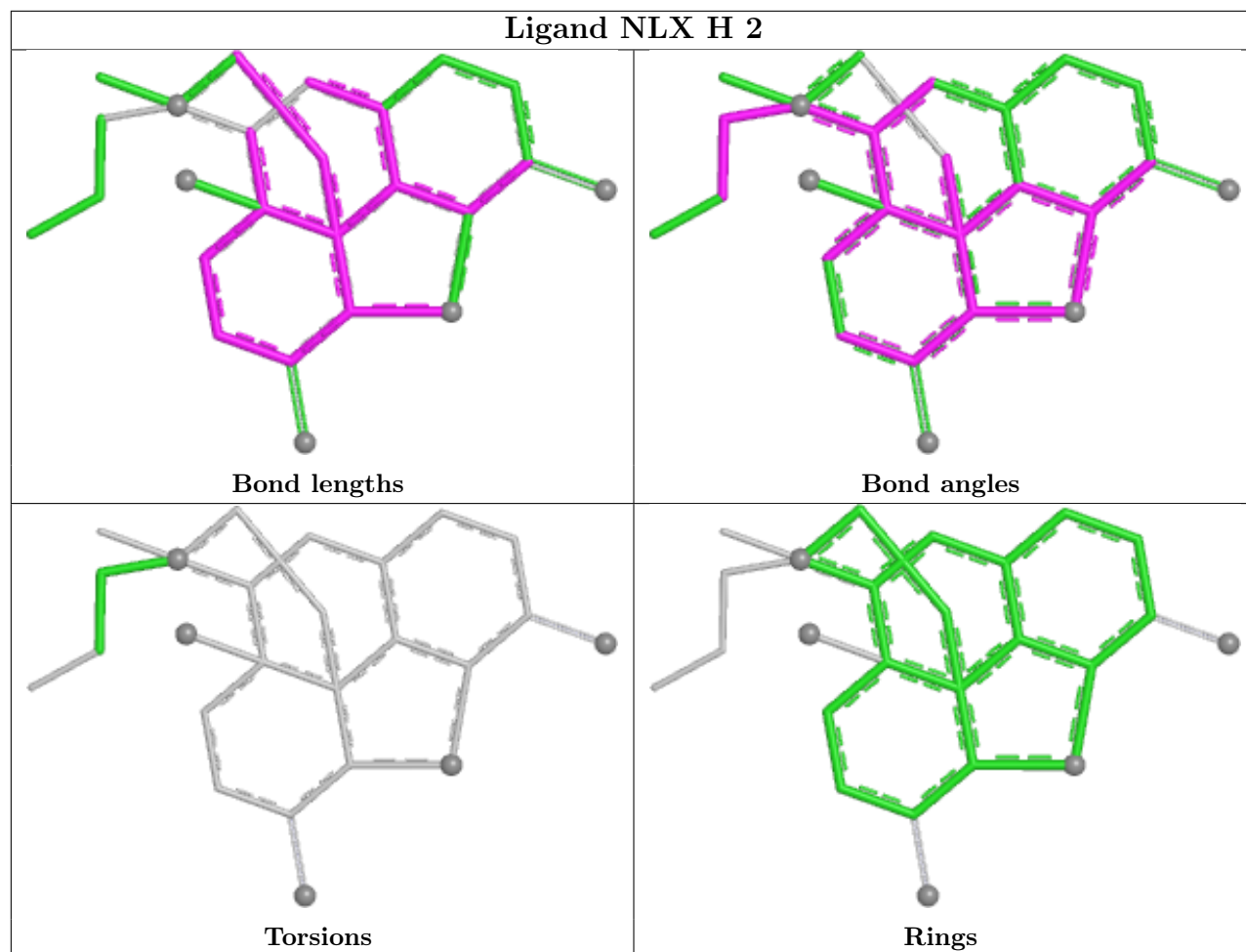


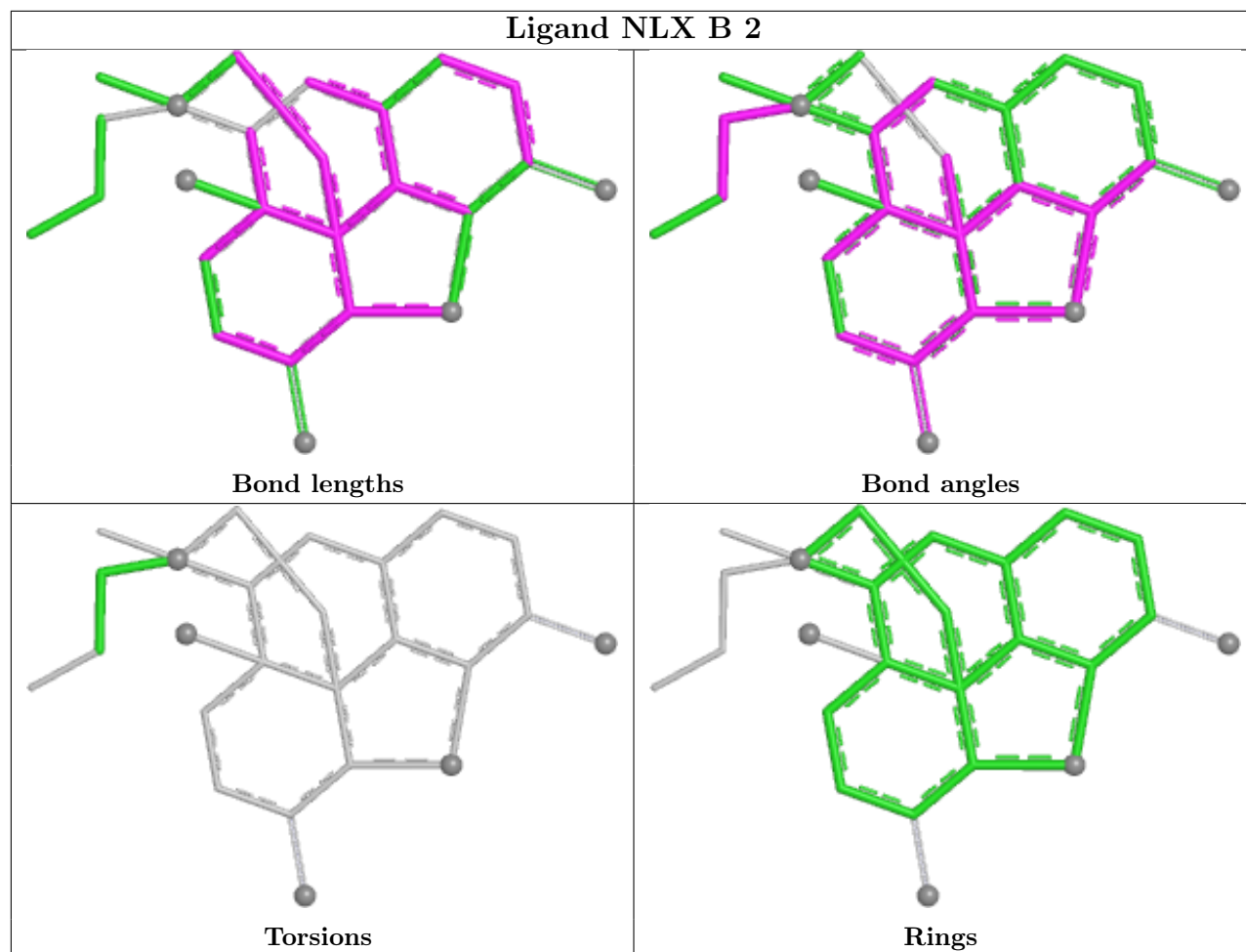












5.7 Other polymers [i](#)

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

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.