



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:59 PM UTC

PDB ID : 2DQZ / pdb_00002dqz
Title : Crystal structure of human carboxylesterase in complex with homatropine, coenzyme A, and palmitate
Authors : Bencharit, S.; Redinbo, M.R.
Deposited on : 2006-06-02
Resolution : 2.80 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)
Xtriage (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

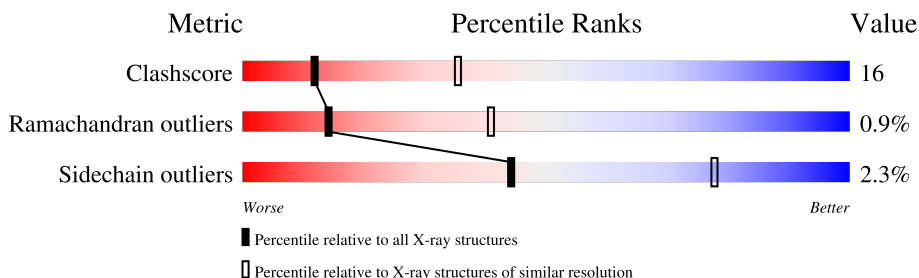
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	542	66% 31% ..
1	B	542	63% 33% ..
1	C	542	70% 27% ..

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	C	379	X	-	-	-
8	COA	C	1	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13161 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.

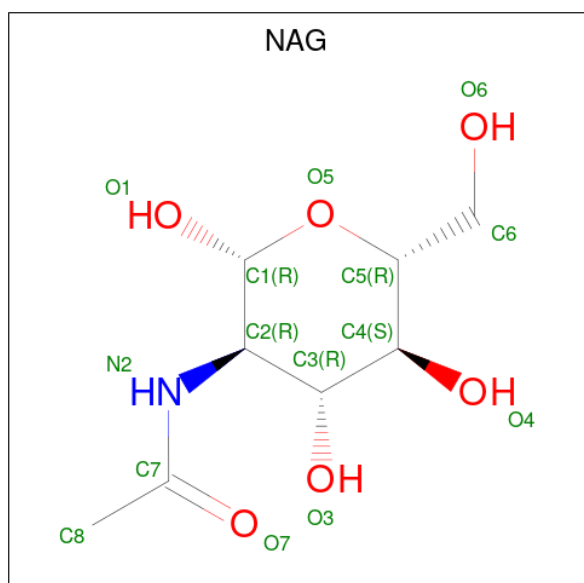
- Molecule 1 is a protein called Liver carboxylesterase 1.

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	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			

There are 3 discrepancies between the modelled and reference sequences:

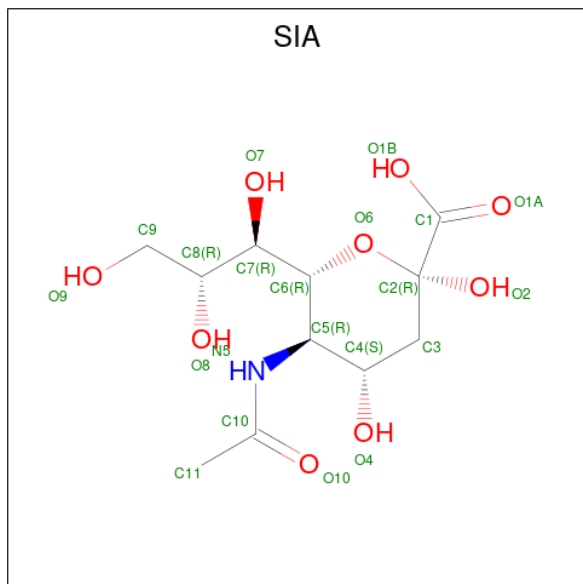
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P23141
B	?	-	GLN	deletion	UNP P23141
C	?	-	GLN	deletion	UNP P23141

- 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	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		

- Molecule 3 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	11	1	9		
3	B	1	Total	C	N	O	0	0
			21	11	1	9		
3	C	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

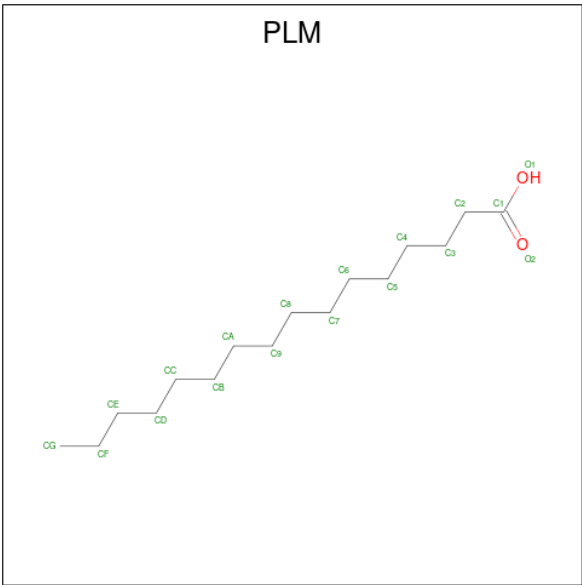


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is FLUORIDE ION (CCD ID: F) (formula: F).

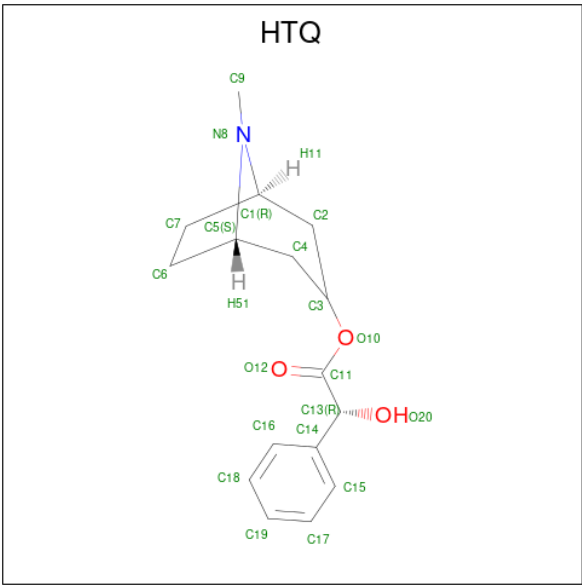
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	F	0	0
			1	1		
5	B	1	Total	F	0	0
			1	1		
5	C	1	Total	F	0	0
			1	1		

- Molecule 6 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	9	2		
6	B	1	Total	C	O	0	0
			11	9	2		
6	C	1	Total	C	O	0	0
			11	9	2		

- Molecule 7 is HOMOTROPINE (CCD ID: HTQ) (formula: C₁₆H₂₁NO₃).



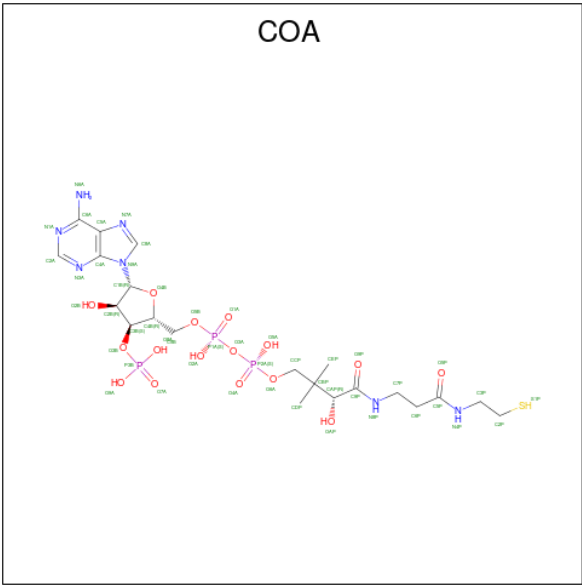
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			20	16	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			20	16	1	3		
7	C	1	Total	C	N	O	0	1
			40	32	2	6		

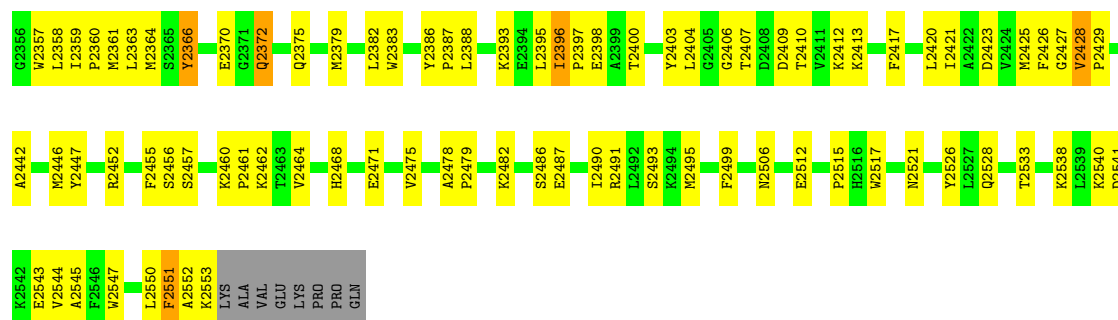
- Molecule 8 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	S	0	0
			7	4	1	1	1		

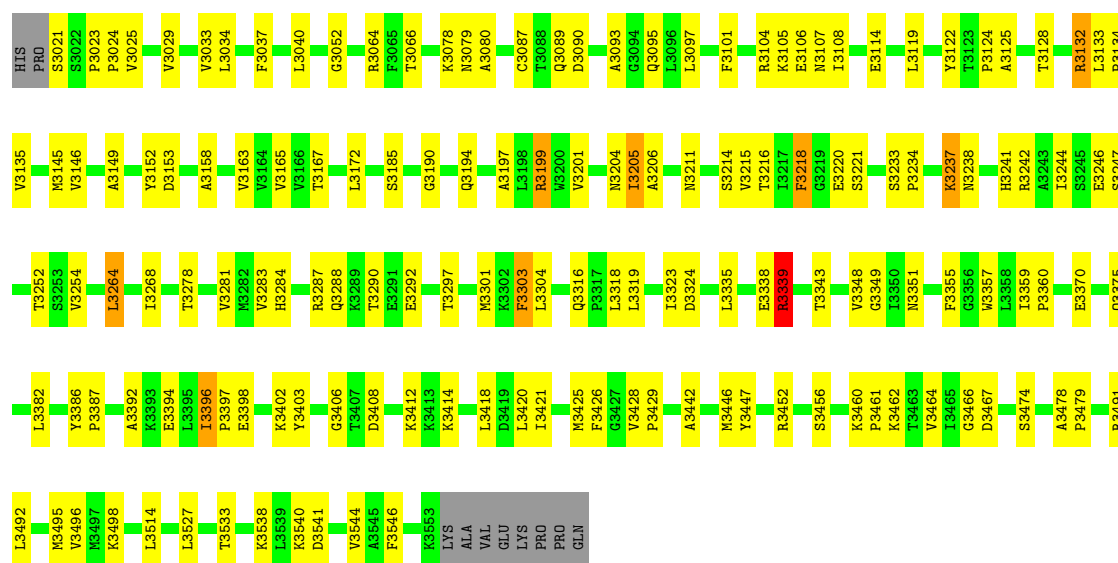
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	179	Total	O	0	0
			179	179		
9	B	135	Total	O	0	0
			135	135		
9	C	194	Total	O	0	0
			194	194		



● Molecule 1: Liver carboxylesterase 1

Chain C: 70% 27% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.56Å 181.02Å 202.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.60 – 2.80	Depositor
% Data completeness (in resolution range)	97.9 (22.60-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.193 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13161	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, F, SIA, SO4, NAG, PLM, HTQ

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	0.47	0/4236	0.90	8/5754 (0.1%)
1	B	0.46	1/4236 (0.0%)	0.89	9/5754 (0.2%)
1	C	0.48	0/4236	0.89	3/5754 (0.1%)
All	All	0.47	1/12708 (0.0%)	0.89	20/17262 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2396	ILE	CA-CB	5.18	1.57	1.54

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1075	SER	N-CA-C	5.95	118.66	111.40
1	B	2114	GLU	N-CA-C	-5.90	105.58	112.89
1	A	1303	PHE	N-CA-C	5.69	117.16	111.07
1	B	2075	SER	N-CA-C	5.68	119.38	112.23
1	B	2303	PHE	N-CA-C	5.67	119.38	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4131	130	0
1	B	4130	0	4131	143	0
1	C	4130	0	4130	116	0
2	A	14	0	13	1	0
2	B	14	0	13	2	0
2	C	14	0	13	1	0
3	A	21	0	18	5	0
3	B	21	0	18	6	0
3	C	21	0	18	4	0
4	A	10	0	0	0	0
4	B	15	0	0	0	0
4	C	10	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	11	0	14	0	0
6	B	11	0	14	2	0
6	C	11	0	14	0	0
7	A	20	0	21	2	0
7	B	20	0	21	0	0
7	C	40	0	42	0	0
8	C	7	0	6	0	0
9	A	179	0	0	17	0
9	B	135	0	0	15	0
9	C	194	0	0	23	0
All	All	13161	0	12617	400	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 16.

The worst 5 of 400 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:C:3292:GLU:HB2	9:C:7340:HOH:O	1.52	1.10
1:A:1199:ARG:HH11	1:A:1199:ARG:HB3	1.22	1.02
1:A:1086:MET:HE2	1:A:1110:LEU:HB2	1.44	0.98
1:C:3134:PRO:HG2	1:C:3163:VAL:HG12	1.45	0.96
1:C:3199:ARG:HH11	1:C:3199:ARG:HB3	1.33	0.93

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	530/542 (98%)	485 (92%)	40 (8%)	5 (1%)	14	41
1	B	530/542 (98%)	477 (90%)	47 (9%)	6 (1%)	11	36
1	C	530/542 (98%)	490 (92%)	36 (7%)	4 (1%)	16	44
All	All	1590/1626 (98%)	1452 (91%)	123 (8%)	15 (1%)	14	41

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2105	LYS
1	A	1320	GLY
1	B	2320	GLY
1	C	3105	LYS
1	C	3406	GLY

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	448/457 (98%)	440 (98%)	8 (2%)	51	82
1	B	448/457 (98%)	434 (97%)	14 (3%)	35	70
1	C	448/457 (98%)	439 (98%)	9 (2%)	48	80
All	All	1344/1371 (98%)	1313 (98%)	31 (2%)	44	78

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2318	LEU
1	C	3218	PHE
1	B	2366	TYR
1	C	3264	LEU
1	C	3132	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2436	ASN
1	B	2534	GLN
1	C	3516	HIS
1	B	2528	GLN
1	C	3107	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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
3	SIA	B	282	-	21,21,21	0.79	0	24,31,31	1.30	3 (12%)
7	HTQ	B	21	-	22,22,22	2.86	13 (59%)	30,31,31	1.77	6 (20%)
7	HTQ	A	11	-	22,22,22	2.99	14 (63%)	30,31,31	1.81	6 (20%)
2	NAG	C	379	1	14,14,15	0.82	0	17,19,21	0.70	0
4	SO4	B	285	-	4,4,4	0.44	0	6,6,6	0.07	0
2	NAG	A	179	1	14,14,15	0.63	0	17,19,21	0.76	0
4	SO4	C	384	-	4,4,4	0.48	0	6,6,6	0.07	0
3	SIA	C	382	-	21,21,21	0.97	2 (9%)	24,31,31	1.78	4 (16%)
2	NAG	B	279	1	14,14,15	0.50	0	17,19,21	0.89	1 (5%)
8	COA	C	1	-	5,6,50	4.43	2 (40%)	5,6,75	4.78	4 (80%)
6	PLM	A	111	-	10,10,17	1.22	2 (20%)	10,10,17	1.12	1 (10%)
4	SO4	B	385	-	4,4,4	0.43	0	6,6,6	0.09	0
6	PLM	B	112	-	10,10,17	1.18	2 (20%)	10,10,17	1.15	2 (20%)
4	SO4	A	284	-	4,4,4	0.38	0	6,6,6	0.11	0
7	HTQ	C	31[A]	-	22,22,22	2.80	13 (59%)	30,31,31	1.90	6 (20%)
4	SO4	B	286	-	4,4,4	0.55	0	6,6,6	0.08	0
6	PLM	C	113	-	10,10,17	1.34	2 (20%)	10,10,17	1.16	1 (10%)
3	SIA	A	182	-	21,21,21	0.96	1 (4%)	24,31,31	1.07	1 (4%)
7	HTQ	C	31[B]	-	22,22,22	2.82	13 (59%)	30,31,31	1.75	6 (20%)
4	SO4	A	184	-	4,4,4	0.52	0	6,6,6	0.11	0
4	SO4	C	185	-	4,4,4	0.46	0	6,6,6	0.04	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
3	SIA	B	282	-	-	5/20/38/38	0/1/1/1
7	HTQ	B	21	-	-	0/12/33/33	0/4/3/3
2	NAG	C	379	1	1/1/5/7	4/6/23/26	0/1/1/1
6	PLM	B	112	-	-	4/8/8/15	-
6	PLM	C	113	-	-	4/8/8/15	-
3	SIA	A	182	-	-	8/20/38/38	0/1/1/1
7	HTQ	C	31[A]	-	-	0/12/33/33	0/4/3/3
3	SIA	C	382	-	-	7/20/38/38	0/1/1/1
2	NAG	B	279	1	-	4/6/23/26	0/1/1/1
7	HTQ	A	11	-	-	1/12/33/33	0/4/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HTQ	C	31[B]	-	-	0/12/33/33	0/4/3/3
6	PLM	A	111	-	-	3/8/8/15	-
2	NAG	A	179	1	-	3/6/23/26	0/1/1/1
8	COA	C	1	-	-	2/4/4/64	-

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1	COA	O5P-C5P	8.11	1.41	1.23
8	C	1	COA	C5P-N4P	5.28	1.48	1.34
7	C	31[A]	HTQ	C9-N8	5.22	1.55	1.47
7	C	31[B]	HTQ	C9-N8	5.14	1.55	1.47
7	B	21	HTQ	C9-N8	5.06	1.54	1.47

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	31[A]	HTQ	C3-O10-C11	7.36	129.29	117.72
8	C	1	COA	O5P-C5P-C6P	-6.69	110.15	122.05
8	C	1	COA	O5P-C5P-N4P	-6.57	104.53	121.78
7	A	11	HTQ	C3-O10-C11	6.46	127.86	117.72
7	B	21	HTQ	C3-O10-C11	6.28	127.59	117.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	379	NAG	C1

5 of 45 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	B	279	NAG	C8-C7-N2-C2
2	B	279	NAG	O7-C7-N2-C2
3	A	182	SIA	O1A-C1-C2-O2

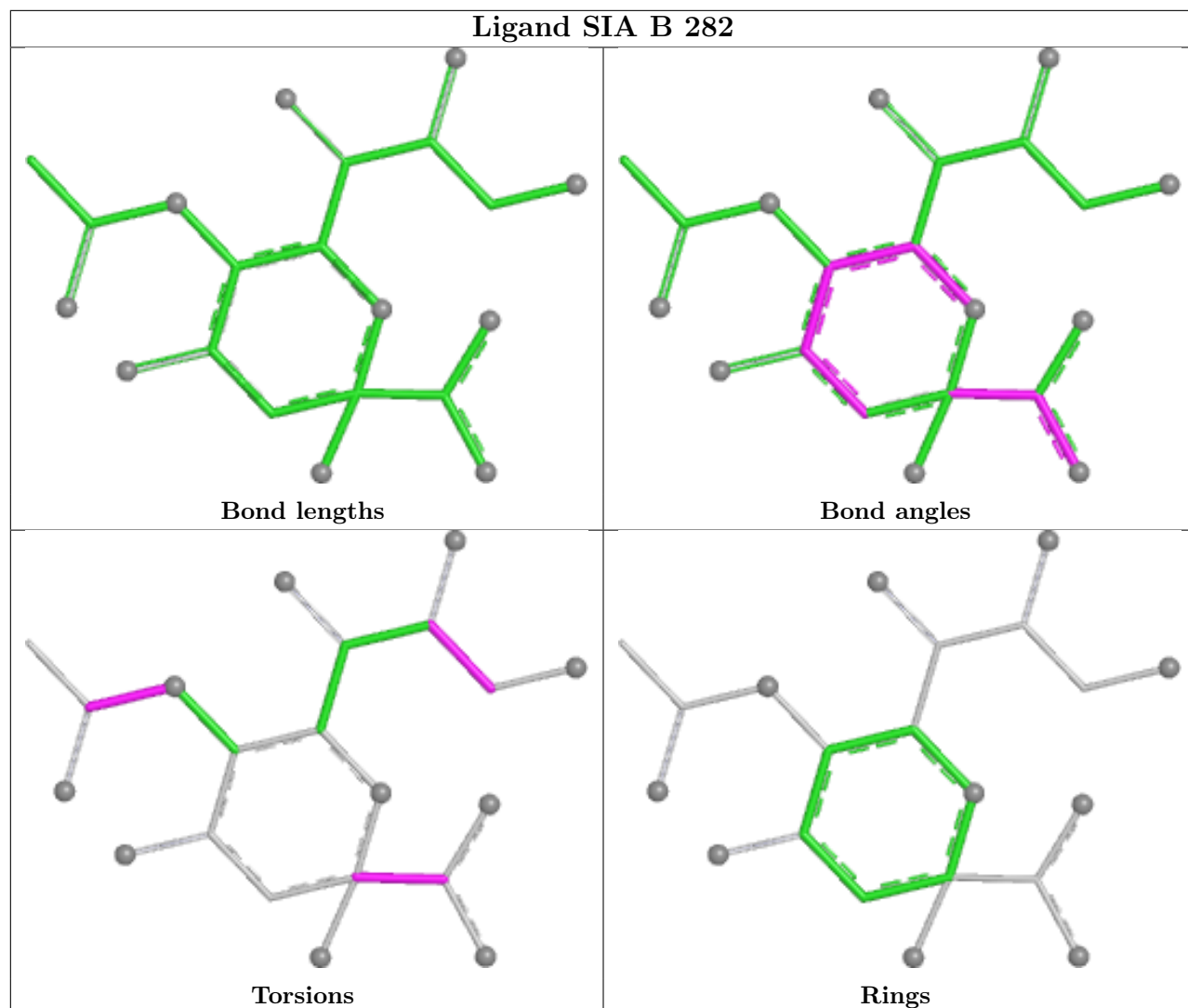
There are no ring outliers.

9 monomers are involved in 22 short contacts:

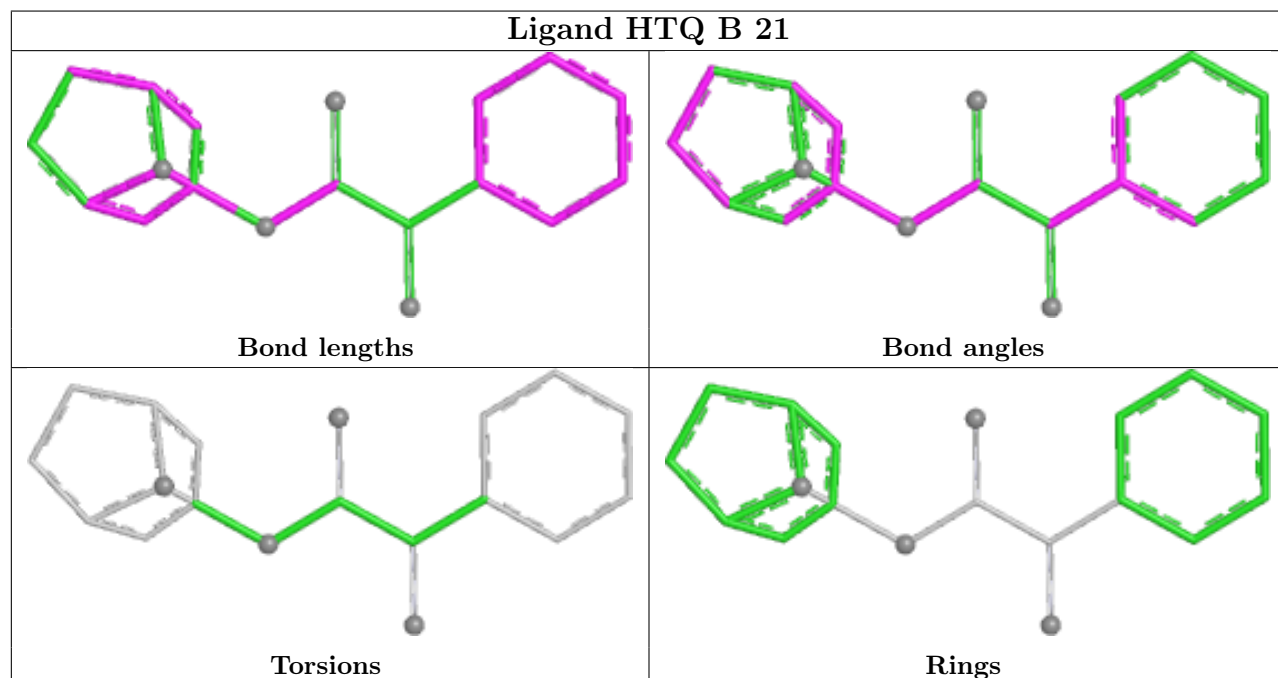
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	282	SIA	6	0
7	A	11	HTQ	2	0
2	C	379	NAG	1	0
2	A	179	NAG	1	0
3	C	382	SIA	4	0
2	B	279	NAG	2	0
6	B	112	PLM	2	0
3	A	182	SIA	5	0
4	C	185	SO4	1	0

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.

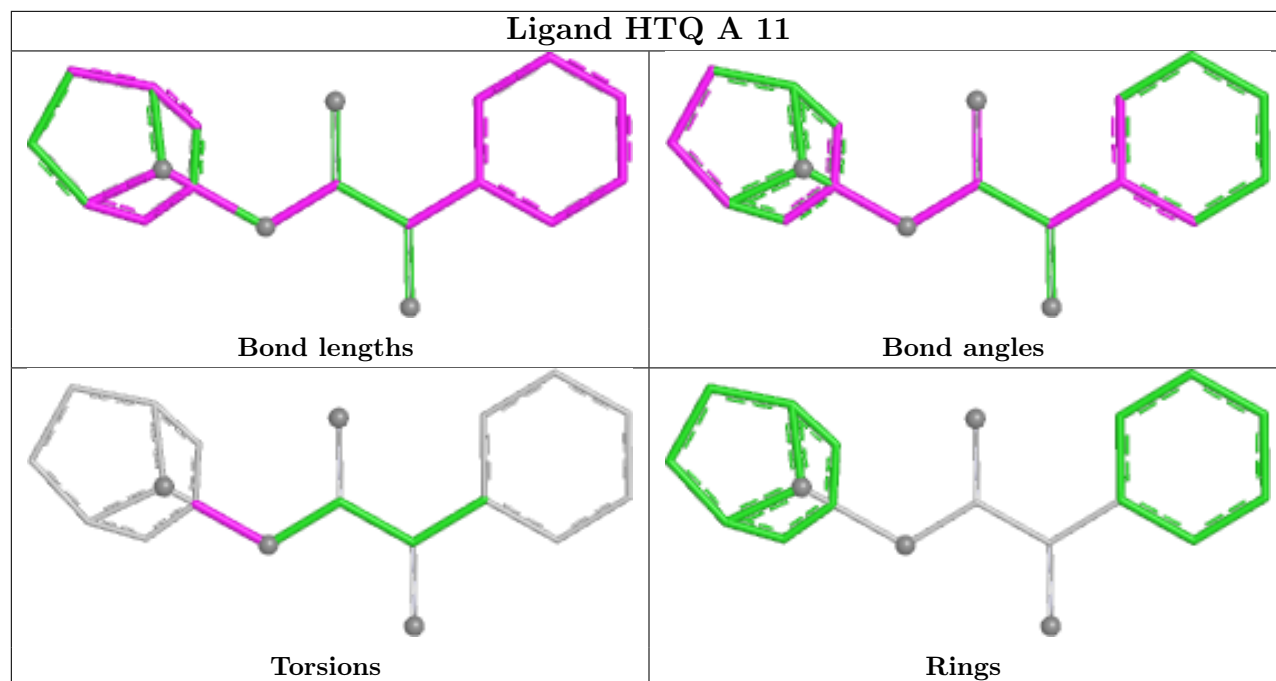
Ligand SIA B 282



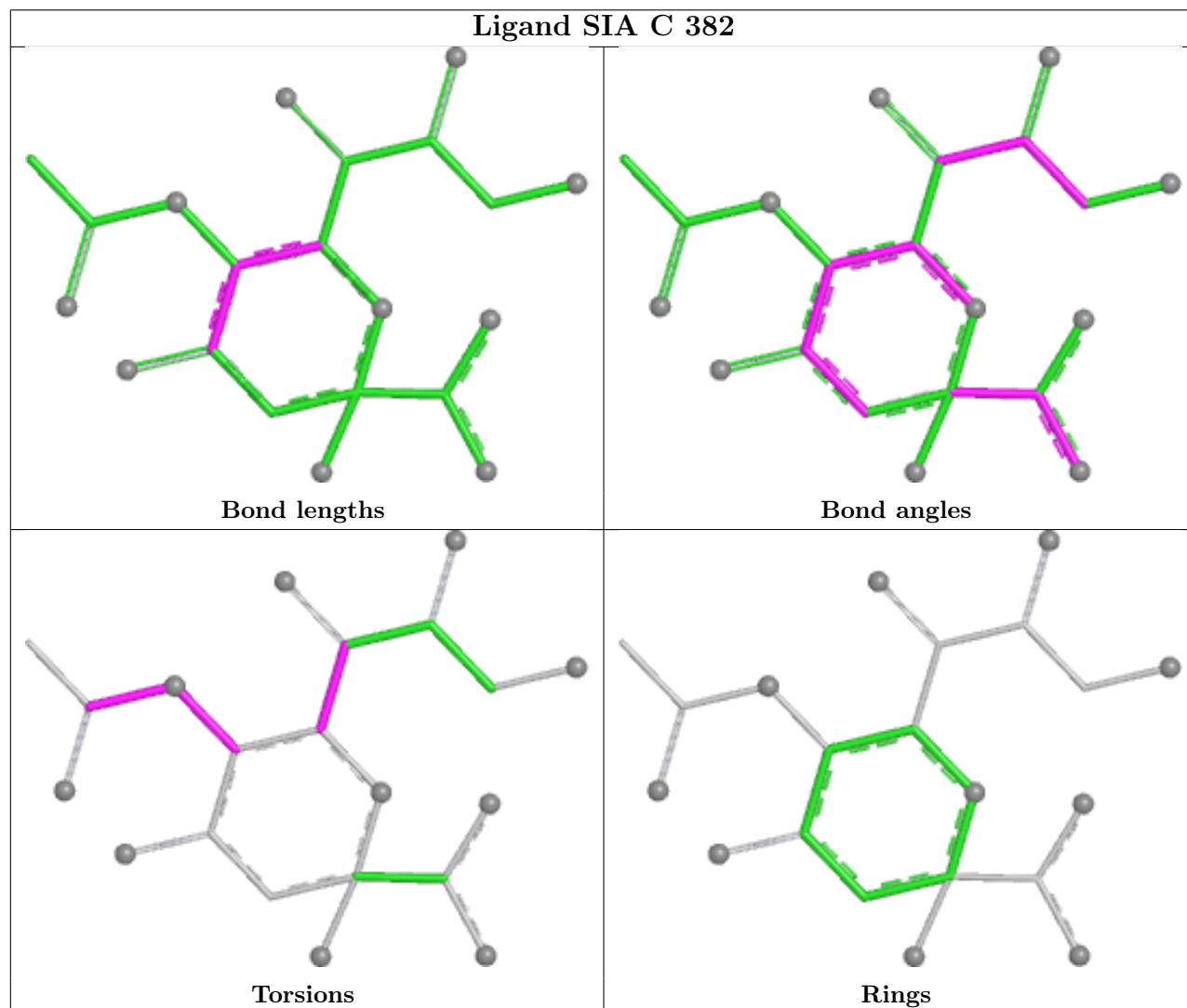
Ligand HTQ B 21

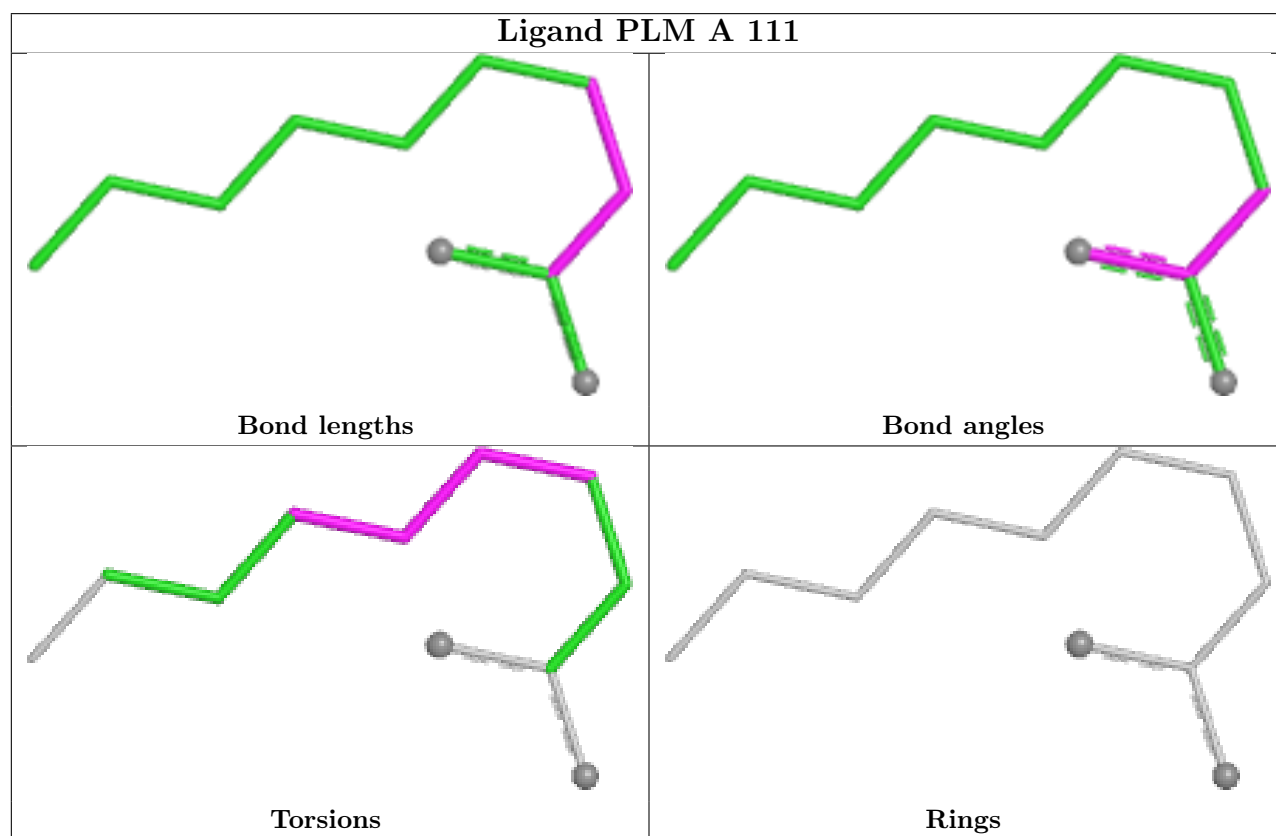
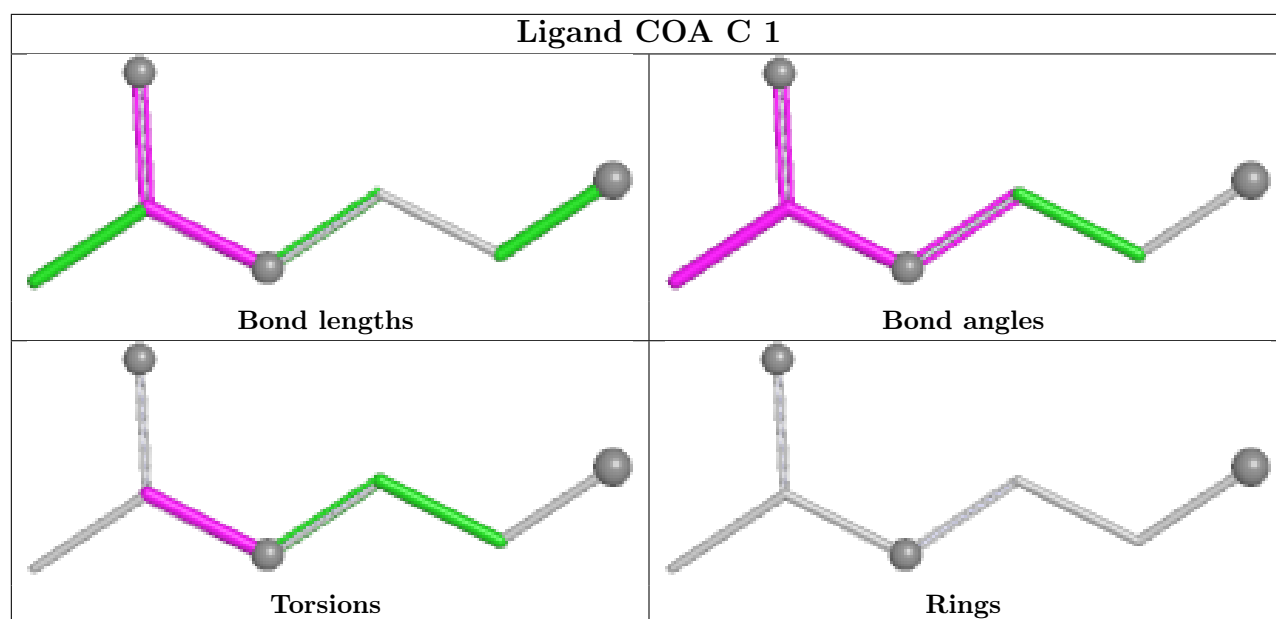


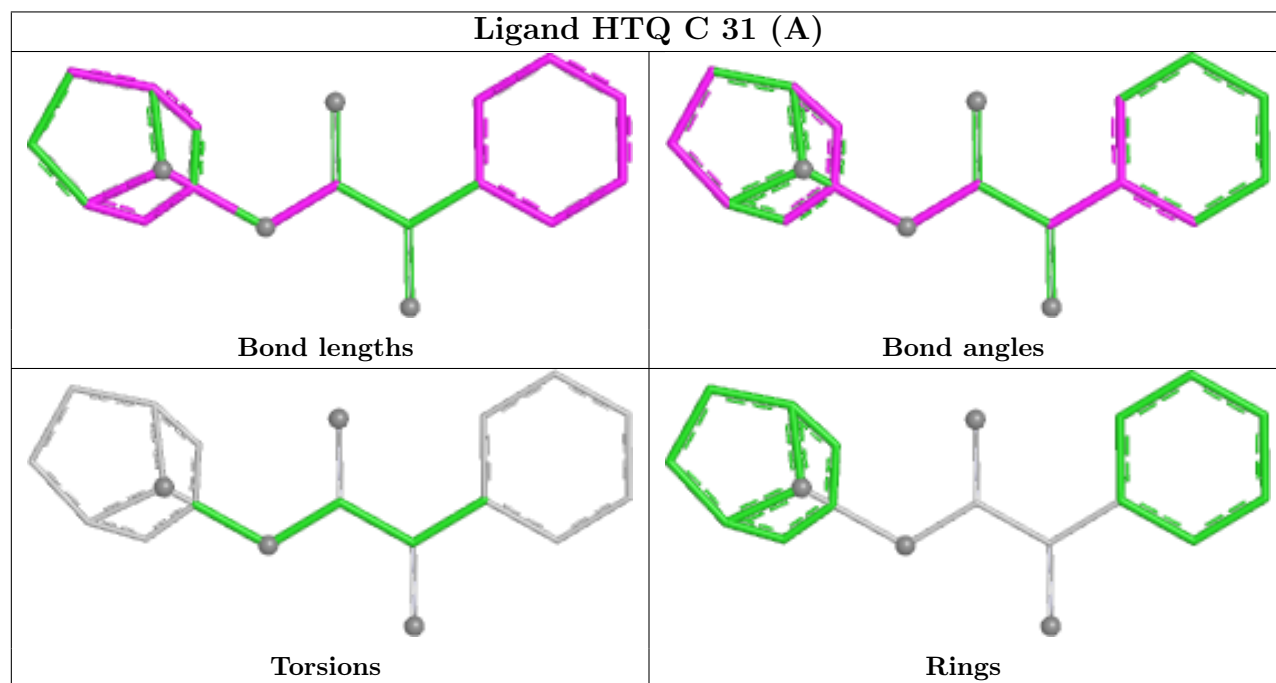
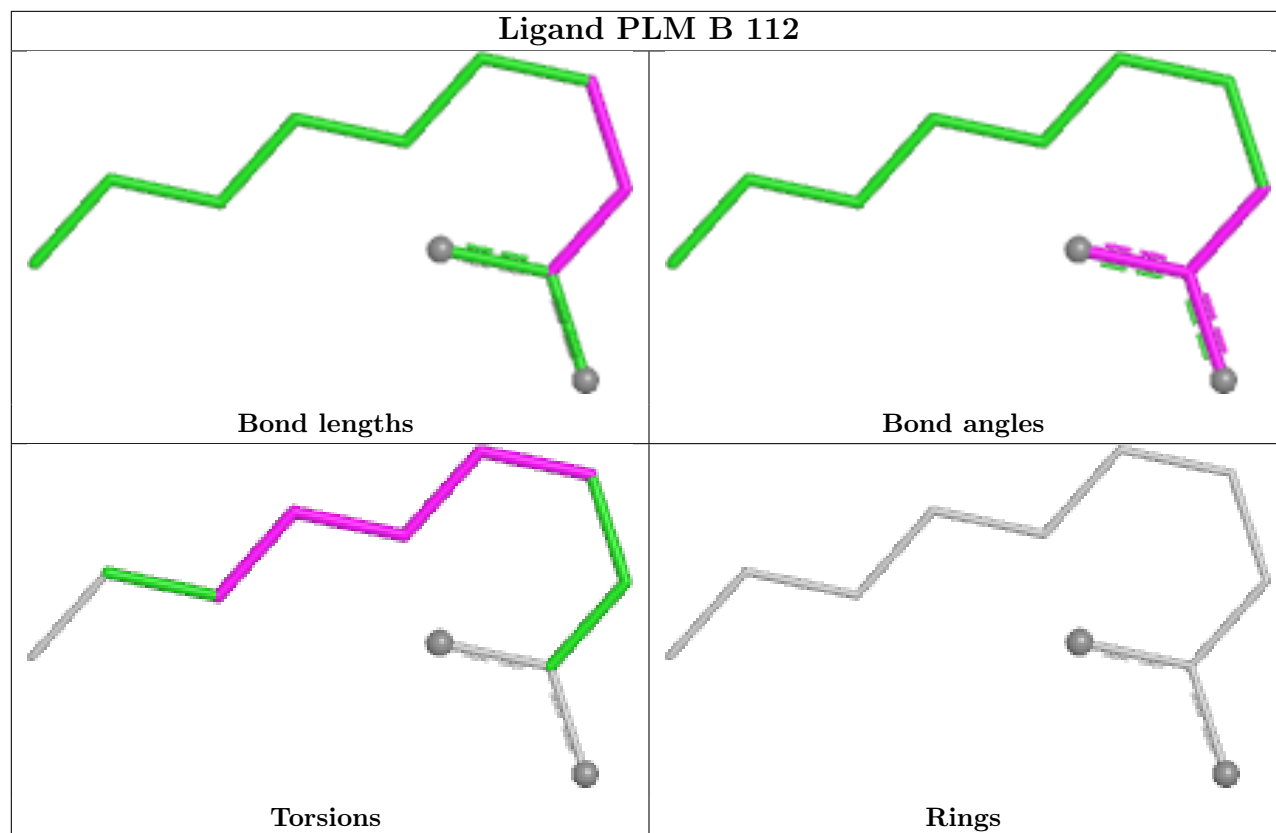
Ligand HTQ A 11

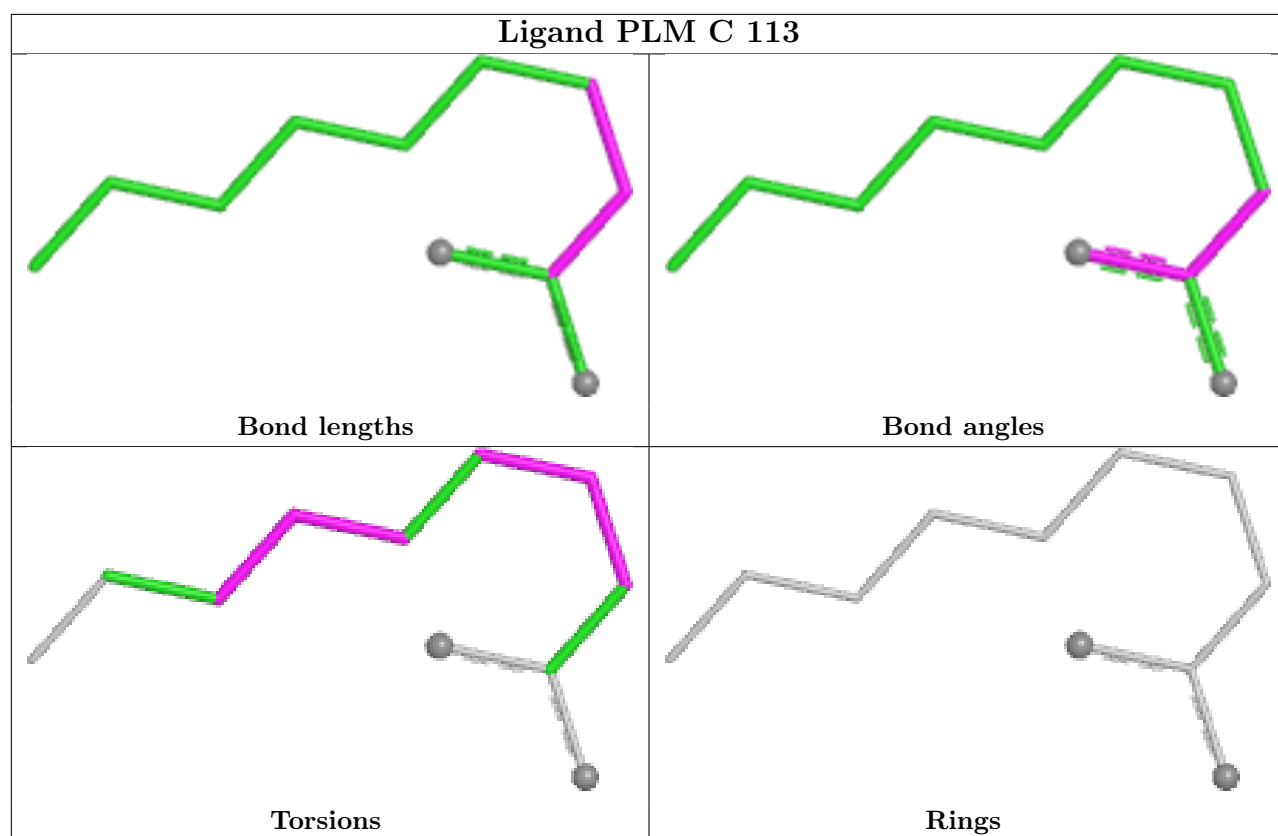


Ligand SIA C 382

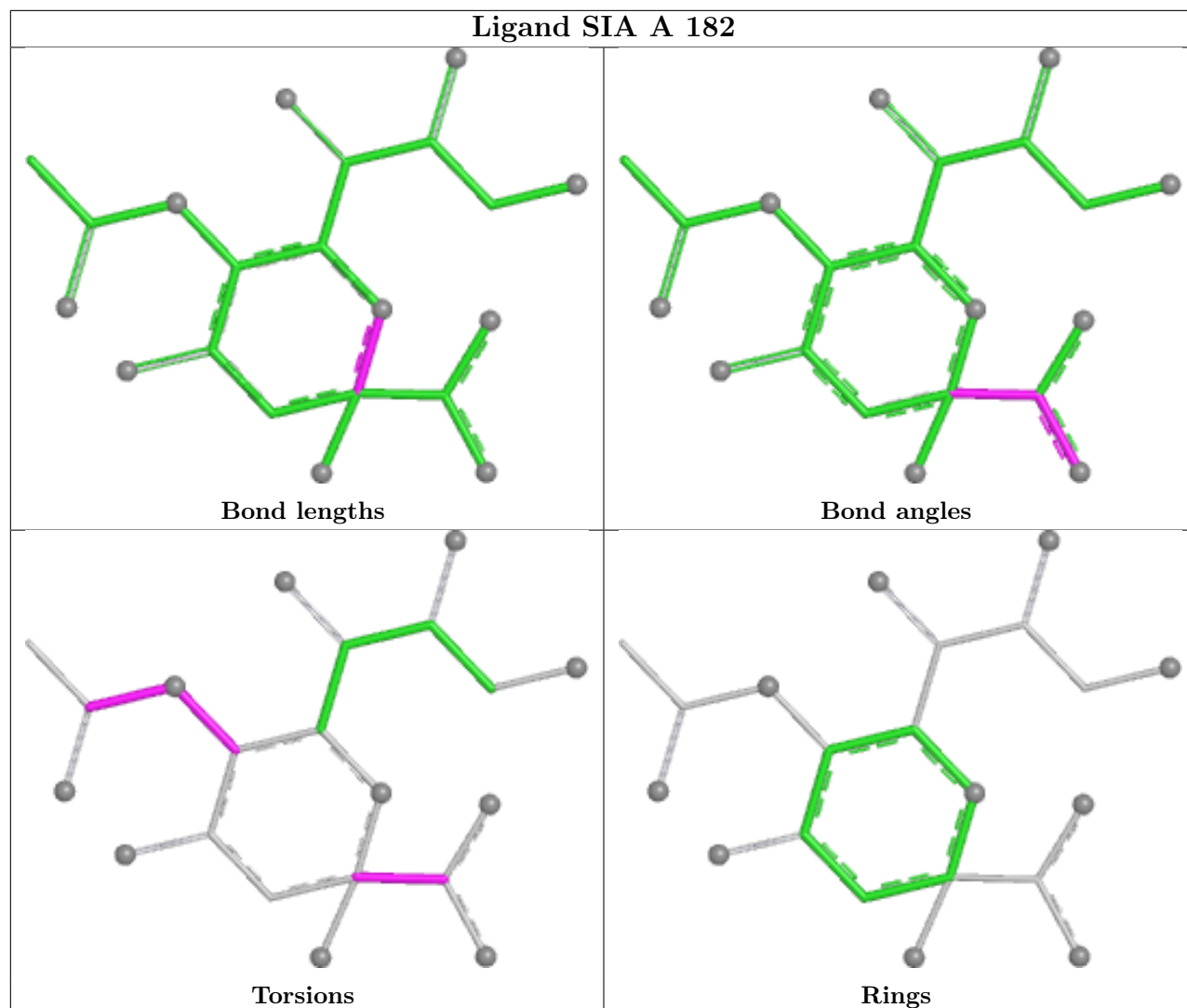




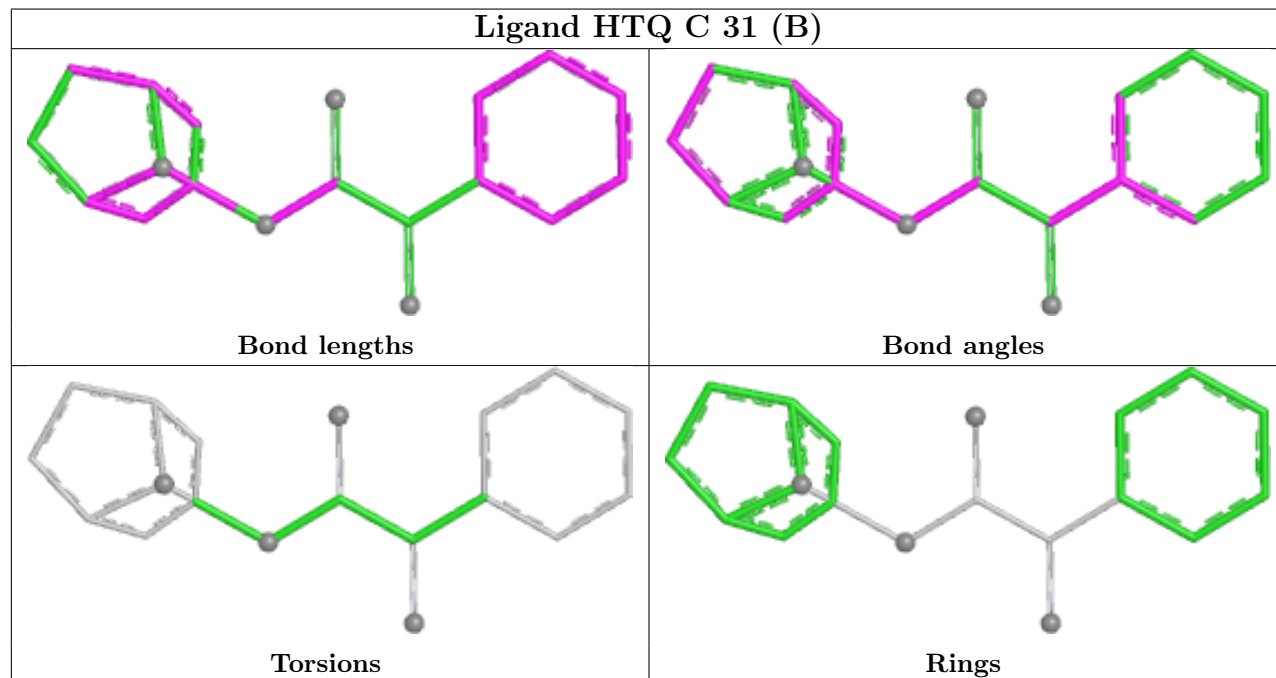




Ligand SIA A 182



Ligand HTQ C 31 (B)



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.