



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 11:09 AM EST

PDB ID : 1MX1
Title : Crystal Structure of Human Liver Carboxylesterase in complex with tacrine
Authors : Bencharit, S.; Morton, C.L.; Hyatt, J.L.; Kuhn, P.; Danks, M.K.; Potter, P.M.; Redinbo, M.R.
Deposited on : 2002-10-01
Resolution : 2.40 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	:	4.02b-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)	:	2.40

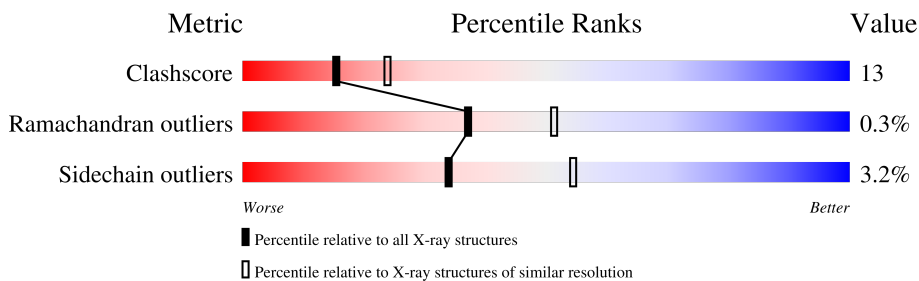
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)

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	
2	G	2	

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
4	SIA	A	1602	-	-	X	-
4	SIA	B	2602	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 27468 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	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	C	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	D	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	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			

There are 6 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
F	?	-	GLN	deletion	UNP P23141

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



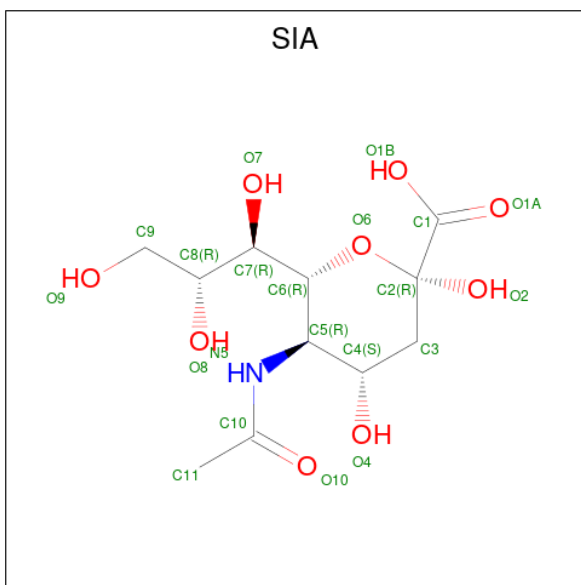
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



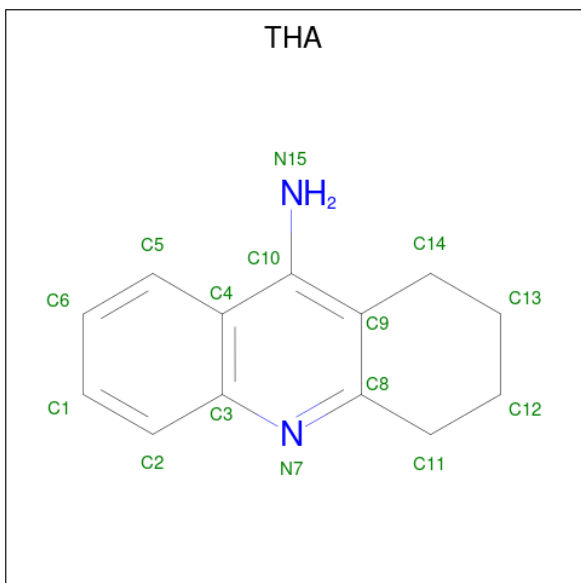
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



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

- Molecule 5 is TACRINE (three-letter code: THA) (formula: $C_{13}H_{14}N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	1
			60	52	8		
5	B	1	Total	C	N	0	1
			60	52	8		
5	C	1	Total	C	N	0	1
			75	65	10		
5	D	1	Total	C	N	0	1
			75	65	10		
5	E	1	Total	C	N	0	1
			75	65	10		
5	F	1	Total	C	N	0	1
			60	52	8		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	374	Total	O	0	0
			374	374		
6	B	359	Total	O	0	0
			359	359		
6	C	362	Total	O	0	0
			362	362		
6	D	306	Total	O	0	0
			306	306		
6	E	357	Total	O	0	0
			357	357		
6	F	359	Total	O	0	0
			359	359		

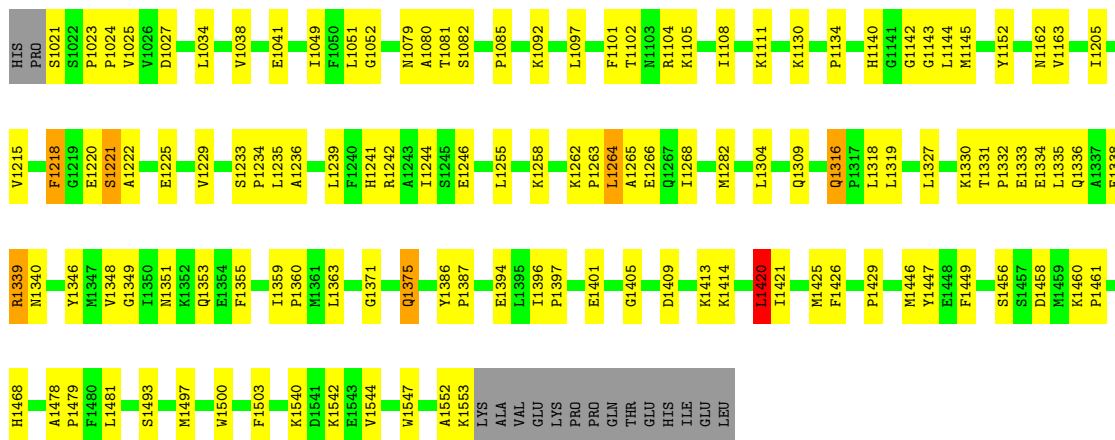
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.


Note EDS was not executed.

• Molecule 1: liver Carboxylesterase I

Chain A: 



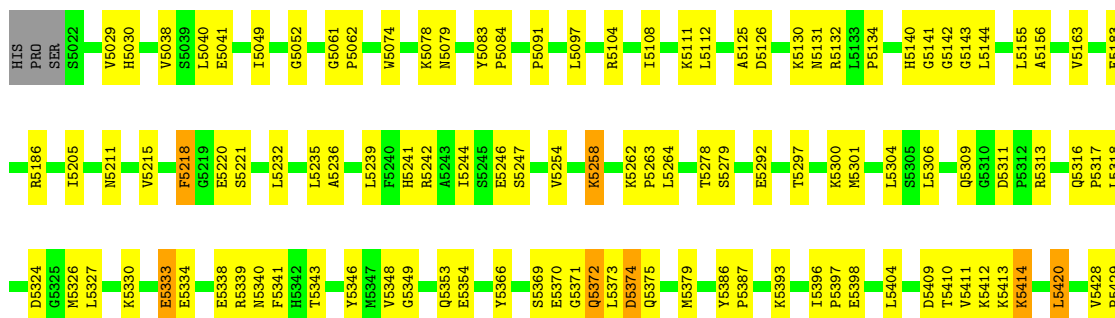
• Molecule 1: liver Carboxylesterase I

Chain B: 



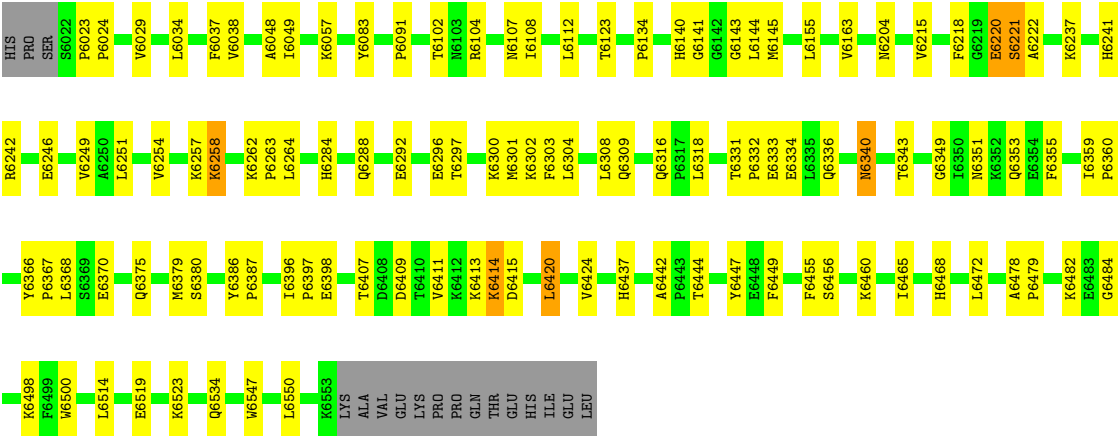
• Molecule 1: liver Carboxylesterase I

Chain C: 

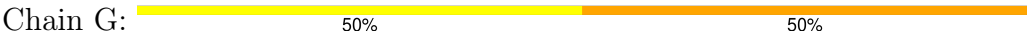




● Molecule 1: liver Carboxylesterase I



● Molecule 2: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.02Å 117.03Å 176.01Å 90.00° 95.69° 90.00°	Depositor
Resolution (Å)	19.98 – 2.40	Depositor
% Data completeness (in resolution range)	99.4 (19.98-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.162 , 0.207	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27468	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: THA, SIA, NDG, 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	0.33	0/4236	0.58	1/5754 (0.0%)
1	B	0.33	0/4230	0.58	0/5746
1	C	0.34	0/4230	0.59	0/5746
1	D	0.32	0/4230	0.56	0/5746
1	E	0.33	0/4230	0.58	0/5746
1	F	0.34	0/4230	0.57	0/5746
All	All	0.33	0/25386	0.58	1/34484 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1420	LEU	CA-CB-CG	5.36	127.63	115.30

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	119	0
1	B	4124	0	4126	106	0
1	C	4124	0	4126	126	0
1	D	4124	0	4126	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4124	0	4125	112	0
1	F	4124	0	4126	97	0
2	G	28	0	24	2	0
3	A	14	0	13	0	0
3	B	14	0	13	3	0
3	D	14	0	13	0	0
3	E	14	0	13	1	0
3	F	28	0	26	1	0
4	A	21	0	18	31	0
4	B	21	0	18	16	0
4	D	21	0	18	7	0
4	E	21	0	18	7	0
5	A	60	0	56	13	0
5	B	60	0	56	9	0
5	C	75	0	70	12	0
5	D	75	0	70	10	0
5	E	75	0	70	14	0
5	F	60	0	56	7	0
6	A	374	0	0	26	0
6	B	359	0	0	15	0
6	C	362	0	0	17	0
6	D	306	0	0	9	0
6	E	357	0	0	22	0
6	F	359	0	0	12	0
All	All	27468	0	25312	672	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 13.

The worst 5 of 672 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:A:1052:GLY:HA3	4:A:1602:SIA:H32	1.24	1.19
4:B:2602:SIA:H111	6:C:3881:HOH:O	1.42	1.18
4:B:2602:SIA:H113	1:C:3278:THR:HB	1.29	1.14
4:A:1602:SIA:H111	1:B:2278:THR:HB	1.31	1.12
1:C:3258:LYS:H	1:C:3258:LYS:HE2	1.09	1.12

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	509 (96%)	20 (4%)	1 (0%)	44	59
1	B	529/548 (96%)	508 (96%)	20 (4%)	1 (0%)	44	59
1	C	529/548 (96%)	509 (96%)	17 (3%)	3 (1%)	22	33
1	D	529/548 (96%)	499 (94%)	28 (5%)	2 (0%)	30	44
1	E	529/548 (96%)	505 (96%)	24 (4%)	0	100	100
1	F	529/548 (96%)	505 (96%)	22 (4%)	2 (0%)	30	44
All	All	3175/3288 (97%)	3035 (96%)	131 (4%)	9 (0%)	37	51

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1339	ARG
1	D	4253	SER
1	C	3185	SER
1	F	6340	ASN
1	B	2357	TRP

5.3.2 Protein sidechains

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%)	437 (98%)	11 (2%)	42	63
1	B	447/463 (96%)	428 (96%)	19 (4%)	25	42
1	C	447/463 (96%)	432 (97%)	15 (3%)	32	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	447/463 (96%)	432 (97%)	15 (3%)	32	52
1	E	447/463 (96%)	433 (97%)	14 (3%)	35	56
1	F	447/463 (96%)	436 (98%)	11 (2%)	42	63
All	All	2683/2778 (97%)	2598 (97%)	85 (3%)	34	54

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4408	ASP
1	E	5414	LYS
1	D	4500	TRP
1	E	5258	LYS
1	F	6218	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	5372	GLN
1	E	5537	GLN
1	F	6351	ASN
1	B	2437	HIS
1	B	2436	ASN

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 ⓘ

2 monosaccharides 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	G	1	2,1	14,14,15	0.76	0	17,19,21	0.68	0
2	NDG	G	2	2	14,14,15	1.13	1 (7%)	17,19,21	1.51	4 (23%)

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	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NDG	G	2	2	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	NDG	O5-C5	3.02	1.49	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NDG	C6-C5-C4	-3.09	105.43	113.02
2	G	2	NDG	C3-C4-C5	2.70	115.12	110.23
2	G	2	NDG	O5-C1-C2	-2.26	107.80	111.29
2	G	2	NDG	C4-C3-C2	-2.03	108.04	111.02

There are no chirality outliers.

All (5) torsion outliers are listed below:

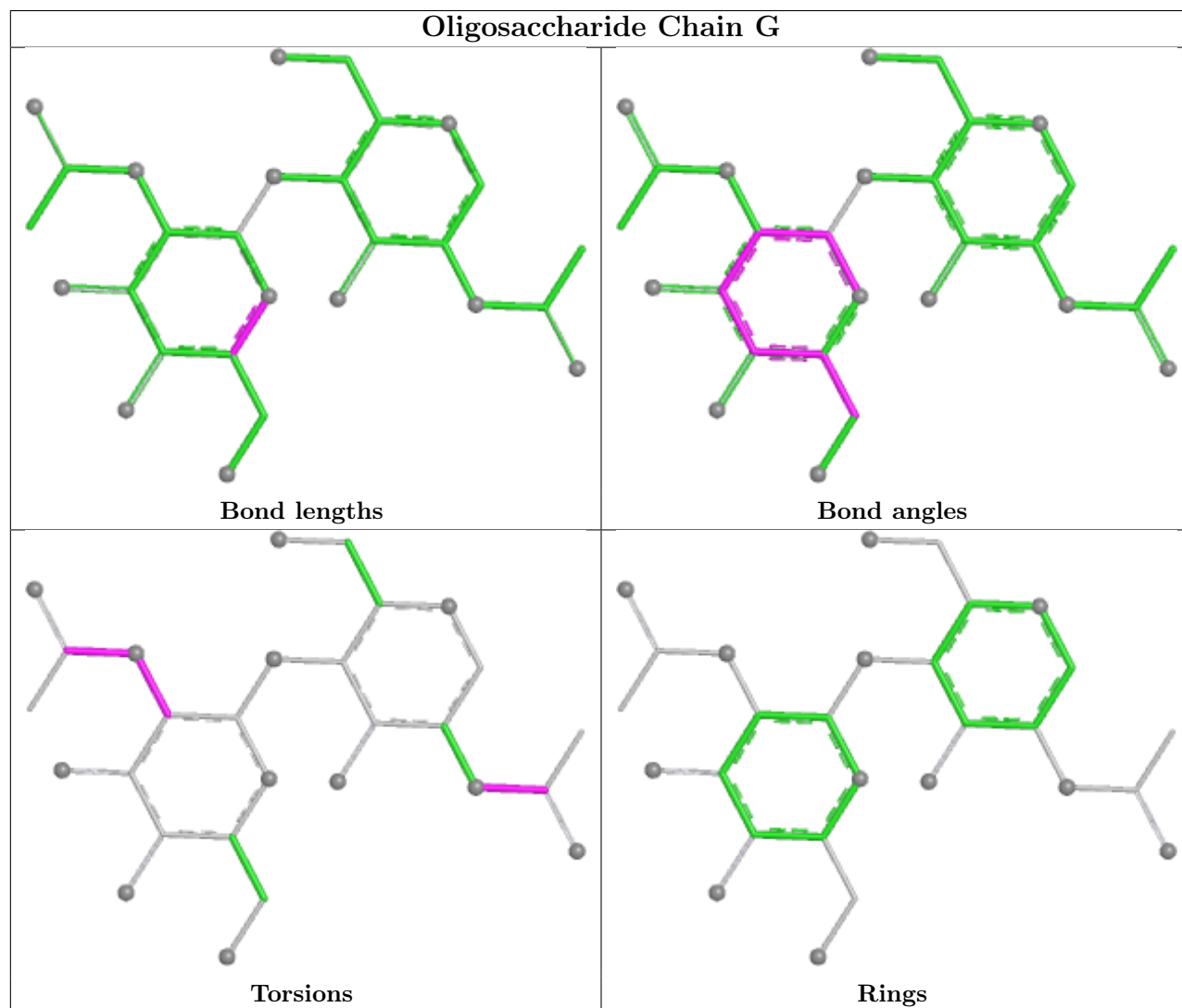
Mol	Chain	Res	Type	Atoms
2	G	2	NDG	C1-C2-N2-C7
2	G	2	NDG	C8-C7-N2-C2
2	G	2	NDG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	2	0
2	G	2	NDG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

37 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$
5	THA	B	2603[A]	-	17,17,17	2.42	7 (41%)	22,24,24	1.70	3 (13%)
5	THA	D	4603[D]	-	17,17,17	2.44	7 (41%)	22,24,24	1.64	3 (13%)
3	NAG	B	2601	1	14,14,15	0.56	0	17,19,21	0.86	1 (5%)
5	THA	B	2603[C]	-	17,17,17	2.39	7 (41%)	22,24,24	1.63	3 (13%)
5	THA	B	2603[B]	-	17,17,17	2.45	7 (41%)	22,24,24	1.63	3 (13%)
4	SIA	E	5602	-	21,21,21	1.04	1 (4%)	24,31,31	1.46	4 (16%)
5	THA	E	5603[B]	-	17,17,17	2.41	7 (41%)	22,24,24	1.63	3 (13%)
5	THA	C	3601[D]	-	17,17,17	2.34	7 (41%)	22,24,24	1.66	3 (13%)
5	THA	E	5603[D]	-	17,17,17	2.44	7 (41%)	22,24,24	1.62	4 (18%)
3	NAG	F	6601	1	14,14,15	0.50	0	17,19,21	0.90	1 (5%)
5	THA	A	1603[A]	-	17,17,17	2.41	7 (41%)	22,24,24	1.64	3 (13%)
5	THA	D	4603[E]	-	17,17,17	2.38	7 (41%)	22,24,24	1.59	3 (13%)
5	THA	F	6603[A]	-	17,17,17	2.40	7 (41%)	22,24,24	1.69	3 (13%)
3	NAG	A	1601	1	14,14,15	0.65	0	17,19,21	0.65	0
3	NAG	F	6602	-	14,14,15	0.50	0	17,19,21	0.67	1 (5%)
5	THA	A	1603[C]	-	17,17,17	2.37	7 (41%)	22,24,24	1.65	3 (13%)
5	THA	D	4603[A]	-	17,17,17	2.43	7 (41%)	22,24,24	1.66	3 (13%)
5	THA	B	2603[D]	-	17,17,17	2.41	7 (41%)	22,24,24	1.59	3 (13%)
5	THA	A	1603[B]	-	17,17,17	2.45	7 (41%)	22,24,24	1.64	3 (13%)
5	THA	F	6603[C]	-	17,17,17	2.36	7 (41%)	22,24,24	1.65	3 (13%)
5	THA	F	6603[B]	-	17,17,17	2.38	7 (41%)	22,24,24	1.59	3 (13%)
5	THA	C	3601[E]	-	17,17,17	2.46	7 (41%)	22,24,24	1.62	4 (18%)
5	THA	D	4603[C]	-	17,17,17	2.42	7 (41%)	22,24,24	1.62	3 (13%)
5	THA	D	4603[B]	-	17,17,17	2.43	7 (41%)	22,24,24	1.60	3 (13%)
4	SIA	B	2602	-	21,21,21	1.04	0	24,31,31	1.13	2 (8%)
5	THA	E	5603[E]	-	17,17,17	2.41	7 (41%)	22,24,24	1.63	3 (13%)
4	SIA	A	1602	-	21,21,21	0.96	1 (4%)	24,31,31	1.34	4 (16%)
5	THA	C	3601[A]	-	17,17,17	2.43	7 (41%)	22,24,24	1.60	3 (13%)
3	NAG	E	5601	1	14,14,15	0.59	0	17,19,21	0.71	1 (5%)
4	SIA	D	4602	-	21,21,21	1.16	1 (4%)	24,31,31	1.16	3 (12%)
5	THA	E	5603[A]	-	17,17,17	2.45	7 (41%)	22,24,24	1.61	3 (13%)
5	THA	C	3601[C]	-	17,17,17	2.43	7 (41%)	22,24,24	1.59	3 (13%)
5	THA	C	3601[B]	-	17,17,17	2.46	7 (41%)	22,24,24	1.67	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	THA	A	1603[D]	-	17,17,17	2.39	7 (41%)	22,24,24	1.59	3 (13%)
5	THA	E	5603[C]	-	17,17,17	2.43	7 (41%)	22,24,24	1.63	3 (13%)
3	NAG	D	4601	1	14,14,15	0.51	0	17,19,21	0.68	1 (5%)
5	THA	F	6603[D]	-	17,17,17	2.39	7 (41%)	22,24,24	1.62	3 (13%)

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
5	THA	B	2603[A]	-	-	-	0/3/3/3
5	THA	D	4603[D]	-	-	-	0/3/3/3
3	NAG	B	2601	1	-	4/6/23/26	0/1/1/1
5	THA	B	2603[C]	-	-	-	0/3/3/3
5	THA	B	2603[B]	-	-	-	0/3/3/3
4	SIA	E	5602	-	-	1/20/38/38	0/1/1/1
5	THA	E	5603[B]	-	-	-	0/3/3/3
5	THA	C	3601[D]	-	-	-	0/3/3/3
5	THA	E	5603[D]	-	-	-	0/3/3/3
3	NAG	F	6601	1	-	2/6/23/26	0/1/1/1
5	THA	A	1603[A]	-	-	-	0/3/3/3
5	THA	D	4603[E]	-	-	-	0/3/3/3
5	THA	F	6603[A]	-	-	-	0/3/3/3
3	NAG	A	1601	1	-	3/6/23/26	0/1/1/1
3	NAG	F	6602	-	-	2/6/23/26	0/1/1/1
5	THA	A	1603[C]	-	-	-	0/3/3/3
5	THA	D	4603[A]	-	-	-	0/3/3/3
5	THA	B	2603[D]	-	-	-	0/3/3/3
5	THA	A	1603[B]	-	-	-	0/3/3/3
5	THA	F	6603[C]	-	-	-	0/3/3/3
5	THA	F	6603[B]	-	-	-	0/3/3/3
5	THA	C	3601[E]	-	-	-	0/3/3/3
5	THA	D	4603[C]	-	-	-	0/3/3/3
5	THA	D	4603[B]	-	-	-	0/3/3/3
4	SIA	B	2602	-	-	1/20/38/38	0/1/1/1
5	THA	E	5603[E]	-	-	-	0/3/3/3
4	SIA	A	1602	-	-	3/20/38/38	0/1/1/1
5	THA	C	3601[A]	-	-	-	0/3/3/3
3	NAG	E	5601	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SIA	D	4602	-	-	2/20/38/38	0/1/1/1
5	THA	E	5603[A]	-	-	-	0/3/3/3
5	THA	C	3601[C]	-	-	-	0/3/3/3
5	THA	C	3601[B]	-	-	-	0/3/3/3
5	THA	A	1603[D]	-	-	-	0/3/3/3
5	THA	E	5603[C]	-	-	-	0/3/3/3
3	NAG	D	4601	1	-	2/6/23/26	0/1/1/1
5	THA	F	6603[D]	-	-	-	0/3/3/3

The worst 5 of 192 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3601[E]	THA	C14-C9	5.27	1.59	1.51
5	B	2603[B]	THA	C14-C9	5.20	1.59	1.51
5	D	4603[B]	THA	C14-C9	5.11	1.59	1.51
5	E	5603[D]	THA	C14-C9	5.10	1.59	1.51
5	C	3601[A]	THA	C14-C9	5.10	1.59	1.51

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	6603[C]	THA	C8-N7-C3	4.78	123.33	117.67
5	D	4603[D]	THA	C8-N7-C3	4.77	123.32	117.67
5	B	2603[A]	THA	C8-N7-C3	4.77	123.31	117.67
5	B	2603[B]	THA	C8-N7-C3	4.75	123.29	117.67
5	E	5603[B]	THA	C8-N7-C3	4.74	123.29	117.67

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2601	NAG	C8-C7-N2-C2
3	B	2601	NAG	O7-C7-N2-C2
3	E	5601	NAG	C8-C7-N2-C2
3	E	5601	NAG	O7-C7-N2-C2
3	B	2601	NAG	O5-C5-C6-O6

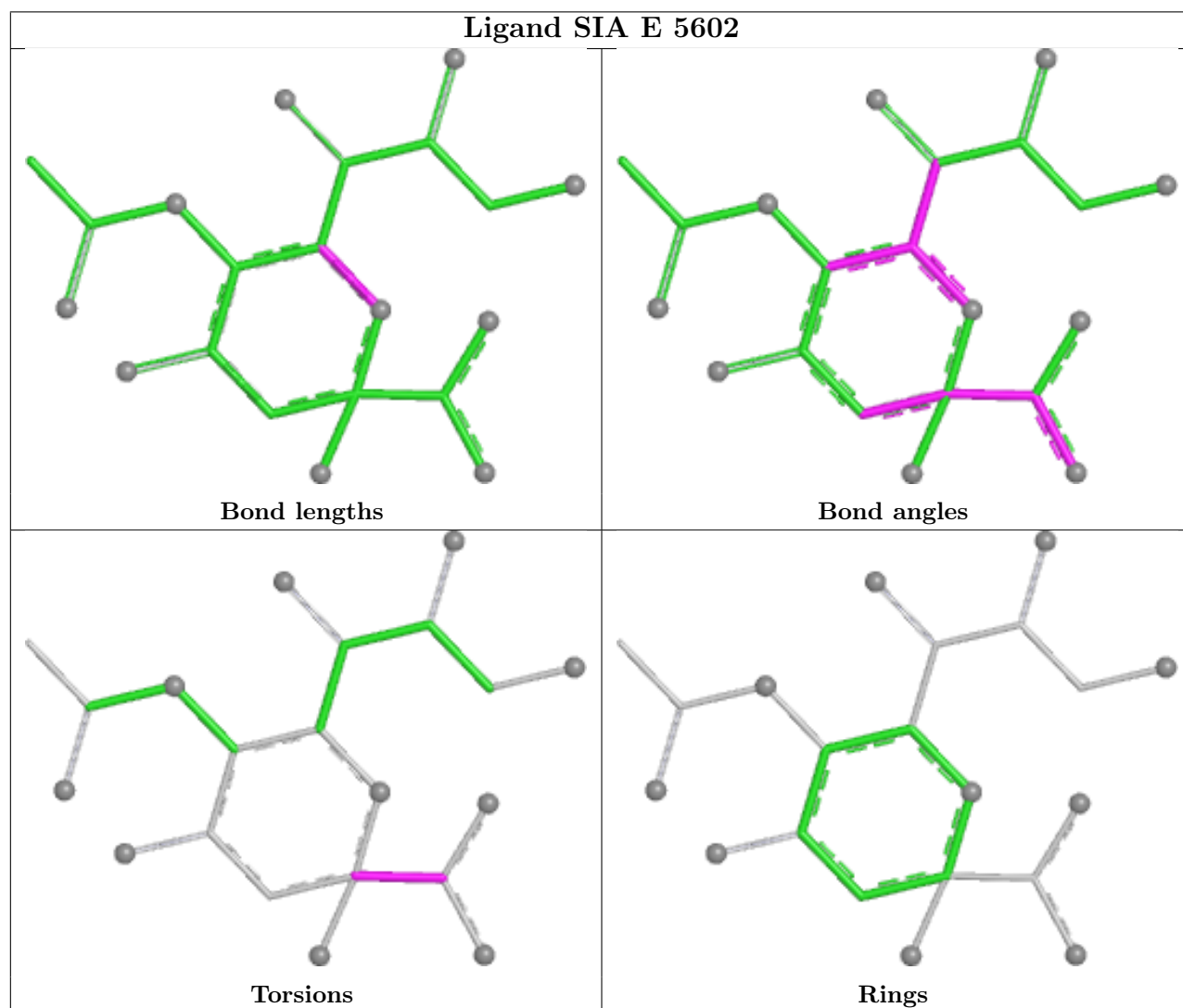
There are no ring outliers.

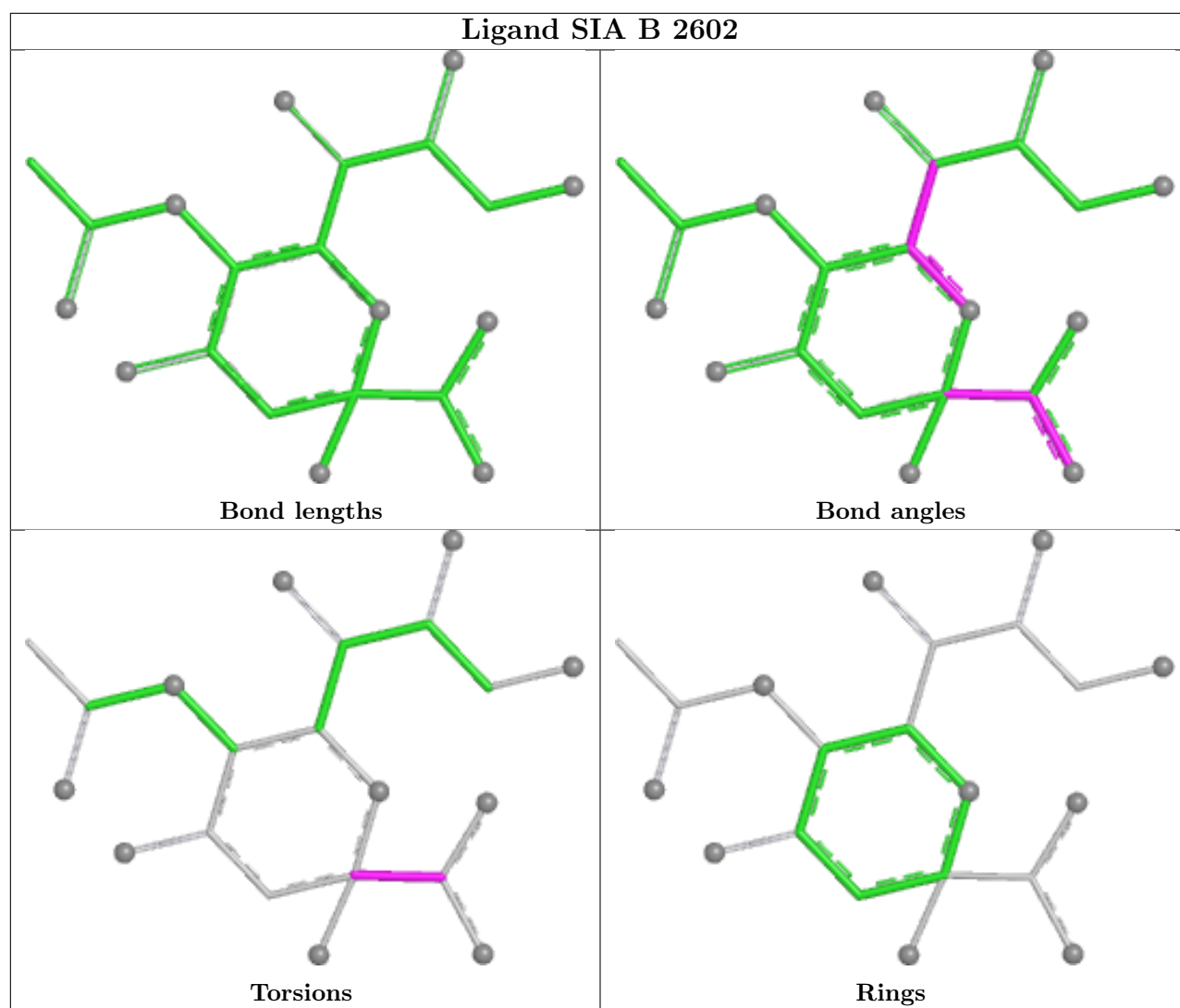
33 monomers are involved in 131 short contacts:

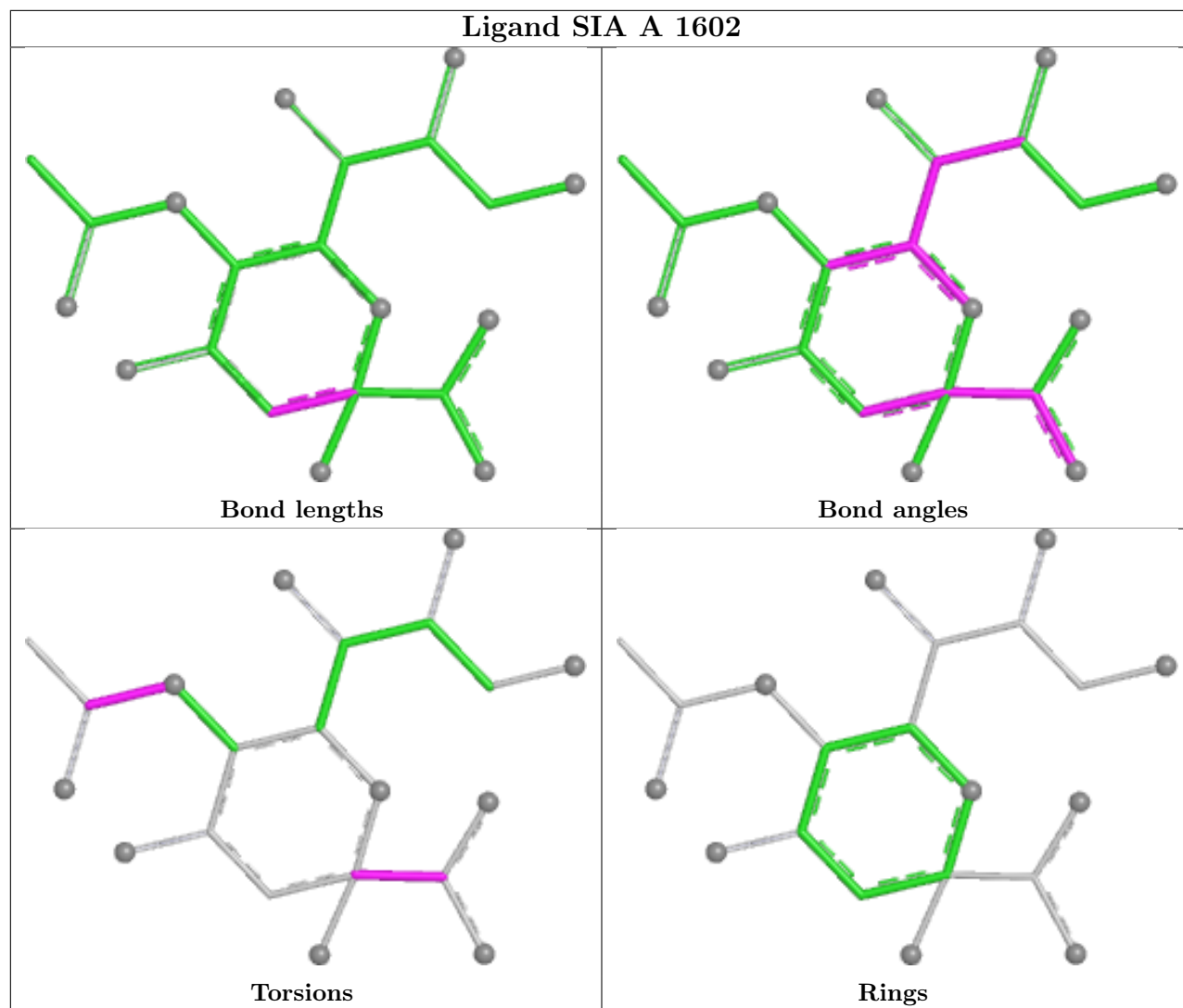
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2603[A]	THA	2	0
3	B	2601	NAG	3	0
5	B	2603[C]	THA	1	0
5	B	2603[B]	THA	5	0
4	E	5602	SIA	7	0
5	E	5603[B]	THA	2	0
5	C	3601[D]	THA	4	0
5	E	5603[D]	THA	3	0
3	F	6601	NAG	1	0
5	A	1603[A]	THA	3	0
5	D	4603[E]	THA	2	0
3	F	6602	NAG	1	0
5	A	1603[C]	THA	4	0
5	D	4603[A]	THA	3	0
5	B	2603[D]	THA	1	0
5	A	1603[B]	THA	3	0
5	F	6603[C]	THA	3	0
5	F	6603[B]	THA	2	0
5	C	3601[E]	THA	3	0
5	D	4603[C]	THA	2	0
5	D	4603[B]	THA	3	0
4	B	2602	SIA	16	0
5	E	5603[E]	THA	4	0
4	A	1602	SIA	31	0
5	C	3601[A]	THA	3	0
3	E	5601	NAG	1	0
4	D	4602	SIA	7	0
5	E	5603[A]	THA	2	0
5	C	3601[C]	THA	1	0
5	C	3601[B]	THA	1	0
5	A	1603[D]	THA	3	0
5	E	5603[C]	THA	3	0
5	F	6603[D]	THA	2	0

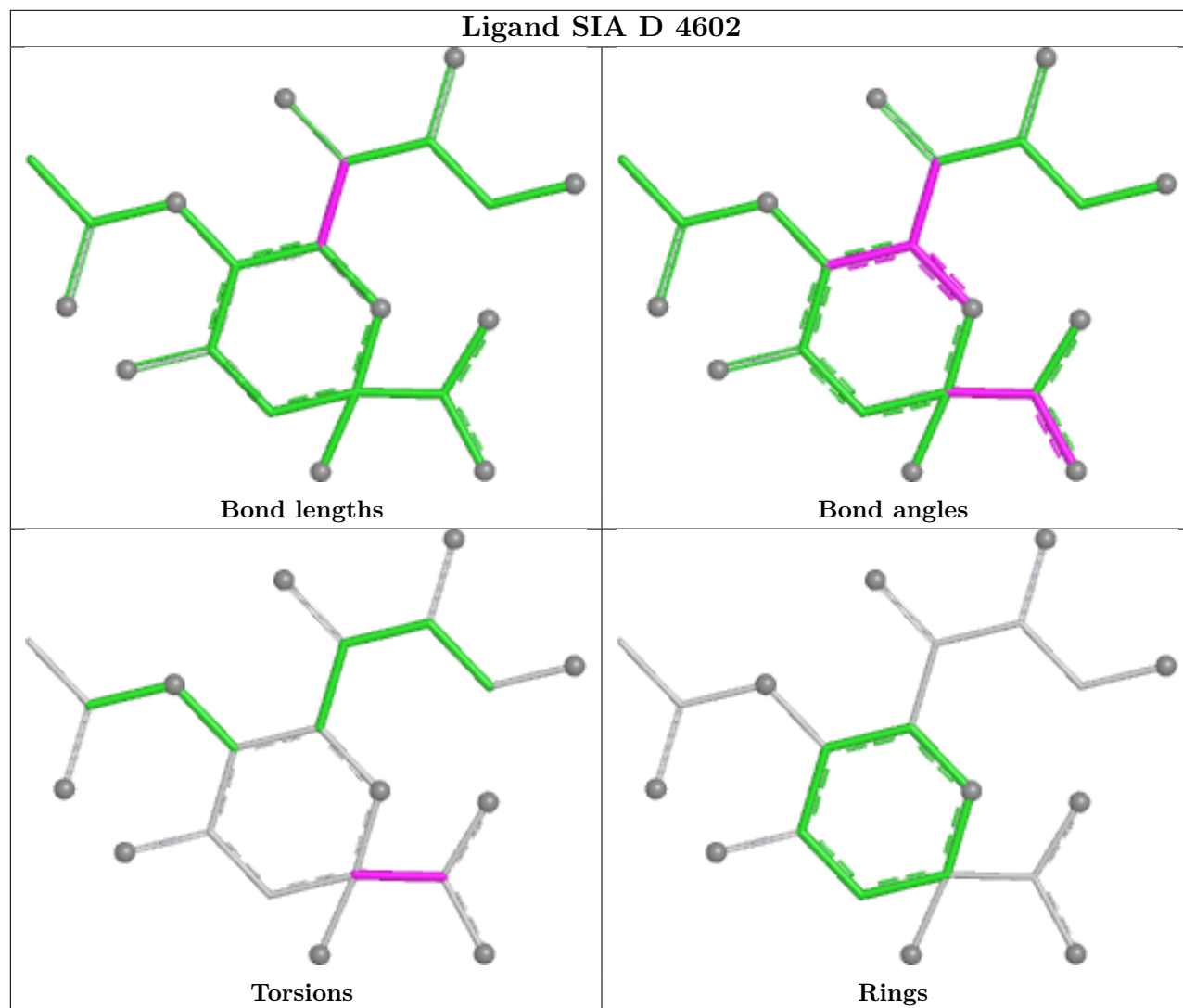
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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