



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 06:39 AM EST

PDB ID : 1ND5  
Title : Crystal Structures of Human Prostatic Acid Phosphatase in Complex with a Phosphate Ion and alpha-Benzylaminobenzylphosphonic Acid Update the Mechanistic Picture and Offer New Insights into Inhibitor Design  
Authors : Ortlund, E.; LaCount, M.W.; Lebioda, L.  
Deposited on : 2002-12-07  
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](mailto: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>.

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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

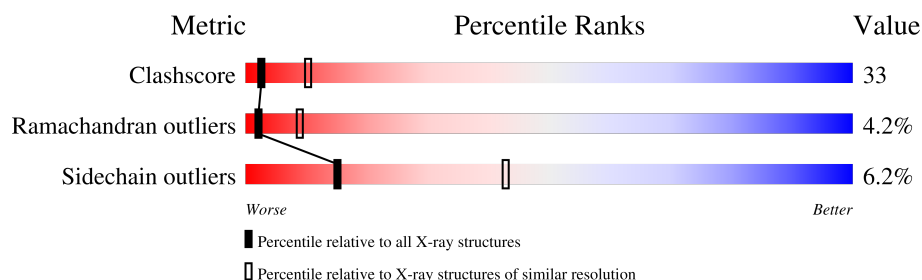
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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  $\geq 3$ , 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	354	44% 47% 6% .
1	B	354	47% 44% 5% .
1	C	354	42% 49% 6% .
1	D	354	43% 47% 6% . .
2	E	2	50% 50%
2	F	2	100%
2	G	2	100%
2	H	2	100%

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Mol	Chain	Length	Quality of chain
3	I	3	

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	E	2	X	-	-	-
2	NAG	F	1	X	-	-	-
2	NAG	G	1	X	-	X	-
2	NAG	H	1	X	-	X	-
2	NAG	H	2	X	-	-	-
3	NAG	I	1	X	-	-	-
4	2BF	D	3402	-	X	-	-
6	NDG	B	1401	-	-	X	-
7	NAG	D	3401	X	-	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11727 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 prostatic acid phosphatase.

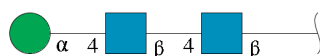
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2800	1807	461	516	16			
1	B	342	Total	C	N	O	S	0	0	0
			2796	1802	461	517	16			
1	C	342	Total	C	N	O	S	0	0	0
			2800	1807	461	516	16			
1	D	342	Total	C	N	O	S	0	0	0
			2800	1807	461	516	16			

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



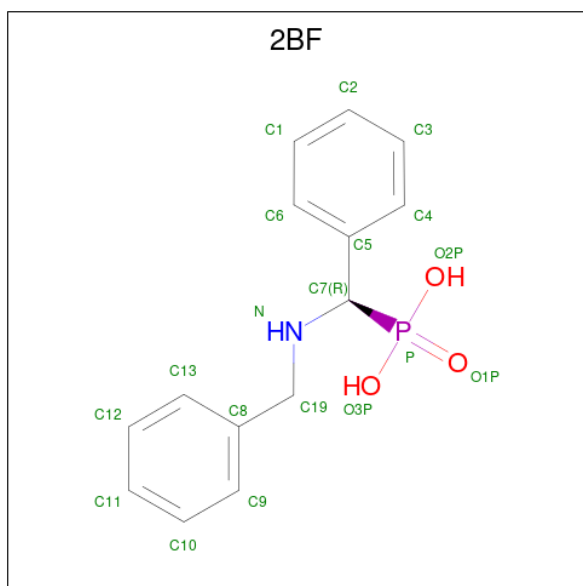
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			30	16	2	12			
2	F	2	Total	C	N	O	0	0	0
			30	16	2	12			
2	G	2	Total	C	N	O	0	0	0
			30	16	2	12			
2	H	2	Total	C	N	O	0	0	0
			30	16	2	12			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	3	Total	C	N	O	0	0	0
			42	22	2	18			

- Molecule 4 is ALPHA-BENZYL-AMINOBENZYL-PHOSPHONIC ACID (three-letter code: 2BF) (formula:  $C_{14}H_{16}NO_3P$ ).



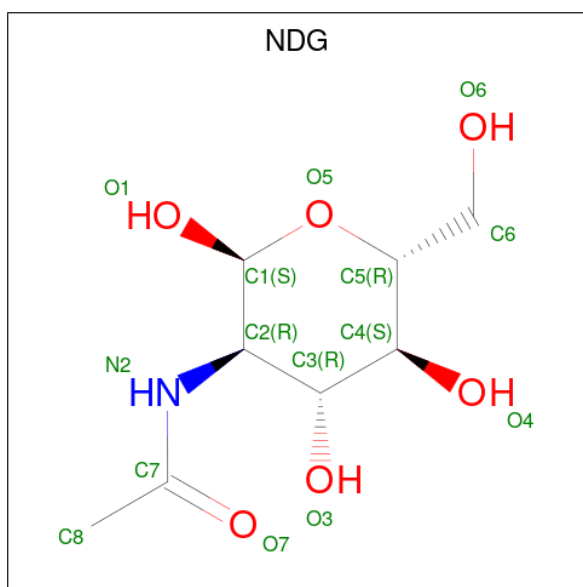
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			19	14	1	3	1		
4	B	1	Total	C	N	O	P	0	0
			19	14	1	3	1		
4	C	1	Total	C	N	O	P	0	0
			19	14	1	3	1		
4	D	1	Total	C	N	O	P	0	0
			19	14	1	3	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	10	6		
5	A	1	Total	C	O	0	0
			16	10	6		
5	A	1	Total	C	O	0	0
			16	10	6		
5	B	1	Total	C	O	0	0
			16	10	6		
5	B	1	Total	C	O	0	0
			16	10	6		
5	C	1	Total	C	O	0	0
			16	10	6		
5	C	1	Total	C	O	0	0
			16	10	6		
5	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 6 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	45	Total 45	O 45	0	0
8	B	35	Total 35	O 35	0	0
8	C	22	Total 22	O 22	0	0
8	D	33	Total 33	O 33	0	0

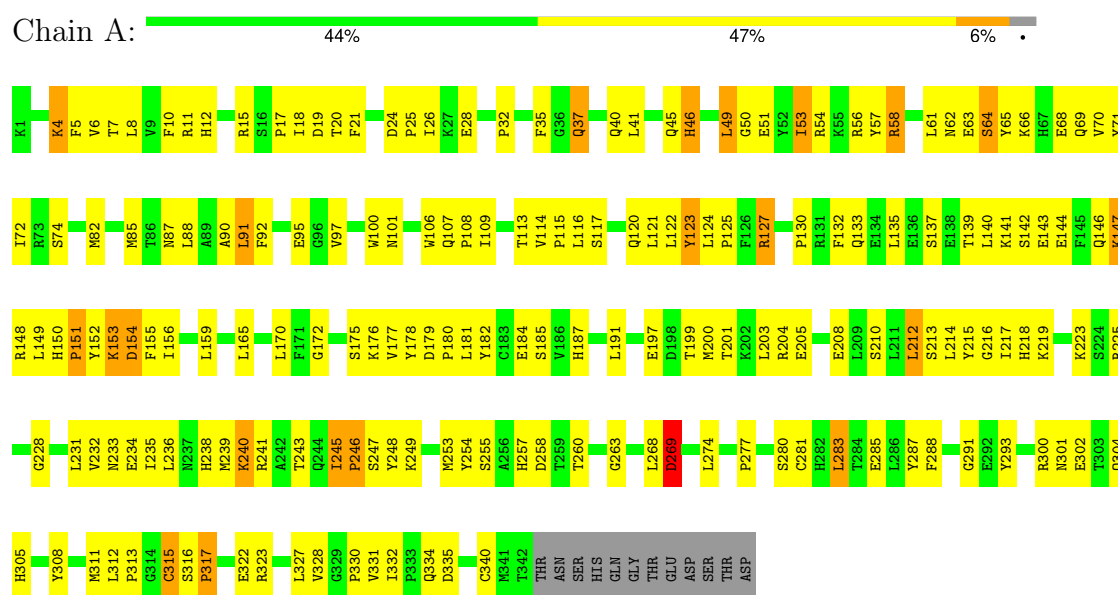


### 3 Residue-property plots

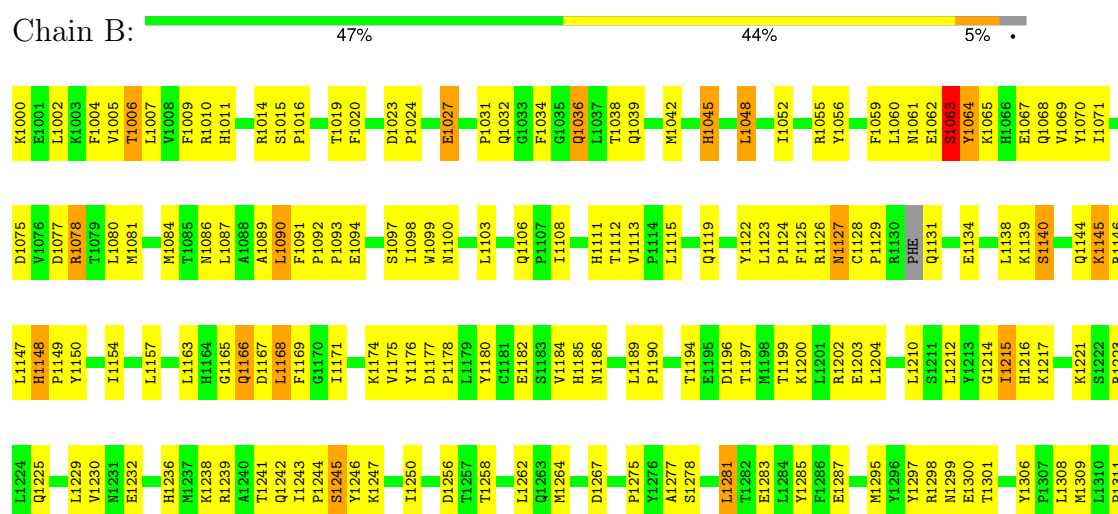
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: prostatic acid phosphatase



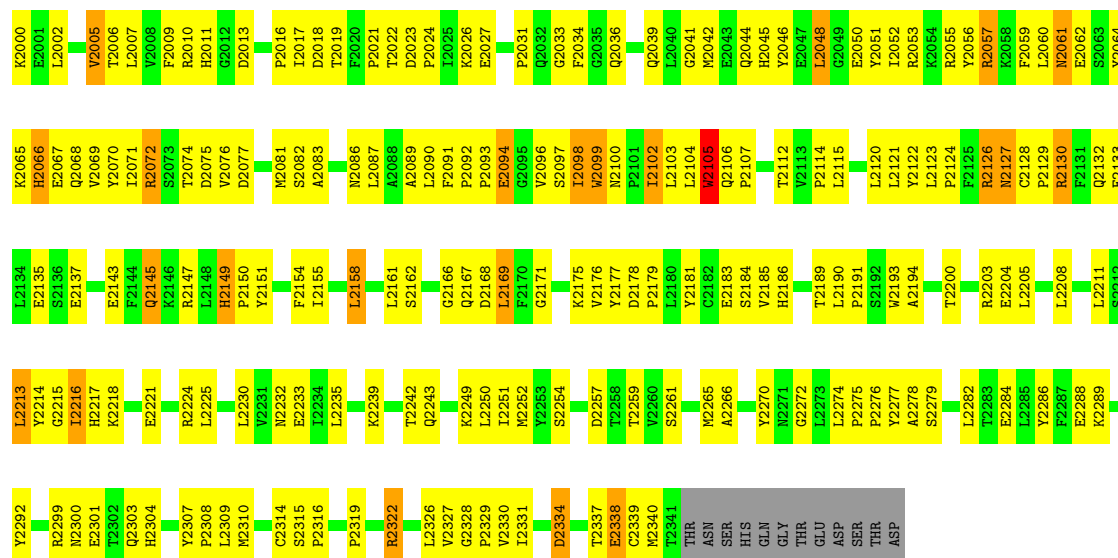
- Molecule 1: prostatic acid phosphatase





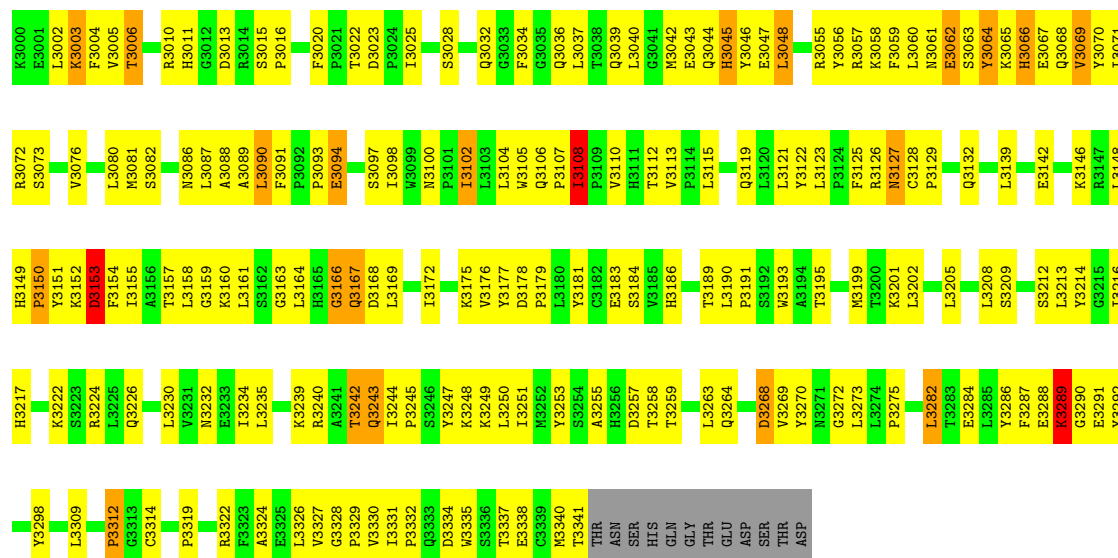
- Molecule 1: prostatic acid phosphatase

Chain C: 42% 49% 6%



- Molecule 1: prostatic acid phosphatase

Chain D: 43% 47% 6%



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

Chain E: 50% 50%

MAG1  
MAG2

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

Chain F:  100%

MAG1  
MAG2

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

Chain G:  100%

MAG1  
MAG2

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

Chain H:  100%

MAG1  
MAG2

- Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33% 33% 33%

MAG1  
MAG2  
MAG3

## 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, $\alpha$ , $\beta$ , $\gamma$	120.10Å 204.86Å 71.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.94 – 2.90	Depositor
% Data completeness (in resolution range)	78.9 (77.94-2.90)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.205 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11727	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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: 2BF, NAG, NDG, 1PE, MAN

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	0/2882	0.64	0/3914
1	B	0.39	0/2876	0.64	0/3905
1	C	0.39	0/2882	0.64	0/3914
1	D	0.39	0/2882	0.62	0/3914
All	All	0.39	0/11522	0.64	0/15647

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2800	0	2749	200	0
1	B	2796	0	2745	177	0
1	C	2800	0	2747	196	0
1	D	2800	0	2746	195	0
2	E	30	0	27	4	0
2	F	30	0	28	4	0
2	G	30	0	28	9	0
2	H	30	0	27	8	0
3	I	42	0	38	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	19	0	14	3	0
4	B	19	0	14	2	0
4	C	19	0	14	2	0
4	D	19	0	14	0	0
5	A	48	0	66	3	0
5	B	32	0	44	5	0
5	C	32	0	44	2	0
5	D	16	0	22	1	0
6	B	15	0	12	7	0
7	D	15	0	14	6	0
8	A	45	0	0	4	0
8	B	35	0	0	4	0
8	C	22	0	0	1	0
8	D	33	0	0	8	0
All	All	11727	0	11393	764	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 33.

The worst 5 of 764 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:I:1:NAG:H61	3:I:2:NAG:H82	1.37	1.07
1:B:1145:LYS:HA	1:B:1145:LYS:HE3	1.32	1.05
1:B:1299:ASN:ND2	2:G:1:NAG:H1	1.74	1.02
1:B:1299:ASN:HD21	2:G:1:NAG:H1	1.23	0.98
1:C:2007:LEU:HD22	1:C:2282:LEU:HD22	1.43	0.97

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	340/354 (96%)	288 (85%)	39 (12%)	13 (4%)	2	11
1	B	338/354 (96%)	284 (84%)	43 (13%)	11 (3%)	3	13
1	C	340/354 (96%)	282 (83%)	41 (12%)	17 (5%)	1	6
1	D	340/354 (96%)	287 (84%)	37 (11%)	16 (5%)	2	7
All	All	1358/1416 (96%)	1141 (84%)	160 (12%)	57 (4%)	2	9

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	65	TYR
1	B	1064	TYR
1	B	1245	SER
1	C	2099	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	314/325 (97%)	293 (93%)	21 (7%)	13	39
1	B	314/325 (97%)	297 (95%)	17 (5%)	18	49
1	C	314/325 (97%)	293 (93%)	21 (7%)	13	39
1	D	314/325 (97%)	295 (94%)	19 (6%)	15	43
All	All	1256/1300 (97%)	1178 (94%)	78 (6%)	15	43

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2230	LEU
1	D	3139	LEU
1	D	3003	LYS
1	D	3062	GLU
1	D	3268	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2186	HIS
1	D	3086	ASN
1	C	2232	ASN
1	D	3045	HIS
1	D	3127	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 ⓘ

11 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	E	1	2,1	15,15,15	0.53	0	21,21,21	0.91	1 (4%)
2	NAG	E	2	2	15,15,15	0.43	0	21,21,21	0.52	0
2	NAG	F	1	2,1	15,15,15	0.42	0	21,21,21	0.69	0
2	NAG	F	2	2	15,15,15	0.45	0	21,21,21	1.07	2 (9%)
2	NAG	G	1	2	15,15,15	0.43	0	21,21,21	0.59	0
2	NAG	G	2	2	15,15,15	0.50	0	21,21,21	1.01	1 (4%)
2	NAG	H	1	2,1	15,15,15	0.74	0	21,21,21	1.04	1 (4%)
2	NAG	H	2	2	15,15,15	0.45	0	21,21,21	0.89	1 (4%)
3	NAG	I	1	1,3	15,15,15	0.54	0	21,21,21	0.58	0
3	NAG	I	2	3	15,15,15	0.47	0	21,21,21	1.05	1 (4%)
3	MAN	I	3	3	12,12,12	0.60	0	17,17,17	0.52	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	E	1	2,1	-	4/6/26/26	0/1/1/1
2	NAG	E	2	2	1/1/6/7	4/6/26/26	0/1/1/1
2	NAG	F	1	2,1	1/1/6/7	2/6/26/26	0/1/1/1
2	NAG	F	2	2	-	2/6/26/26	0/1/1/1
2	NAG	G	1	2	1/1/6/7	2/6/26/26	0/1/1/1
2	NAG	G	2	2	-	4/6/26/26	0/1/1/1
2	NAG	H	1	2,1	1/1/6/7	6/6/26/26	0/1/1/1
2	NAG	H	2	2	1/1/6/7	3/6/26/26	0/1/1/1
3	NAG	I	1	1,3	1/1/6/7	0/6/26/26	0/1/1/1
3	NAG	I	2	3	-	2/6/26/26	0/1/1/1
3	MAN	I	3	3	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	NAG	O1-C1-C2	-3.52	101.91	109.22
3	I	2	NAG	O1-C1-C2	-3.49	101.96	109.22
2	H	1	NAG	C1-C2-C3	-3.30	106.05	110.54
2	G	2	NAG	O1-C1-C2	-3.28	102.41	109.22
2	E	1	NAG	O1-C1-C2	-2.92	103.16	109.22

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	2	NAG	C1
2	F	1	NAG	C1
2	G	1	NAG	C1
2	H	1	NAG	C1
2	H	2	NAG	C1

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

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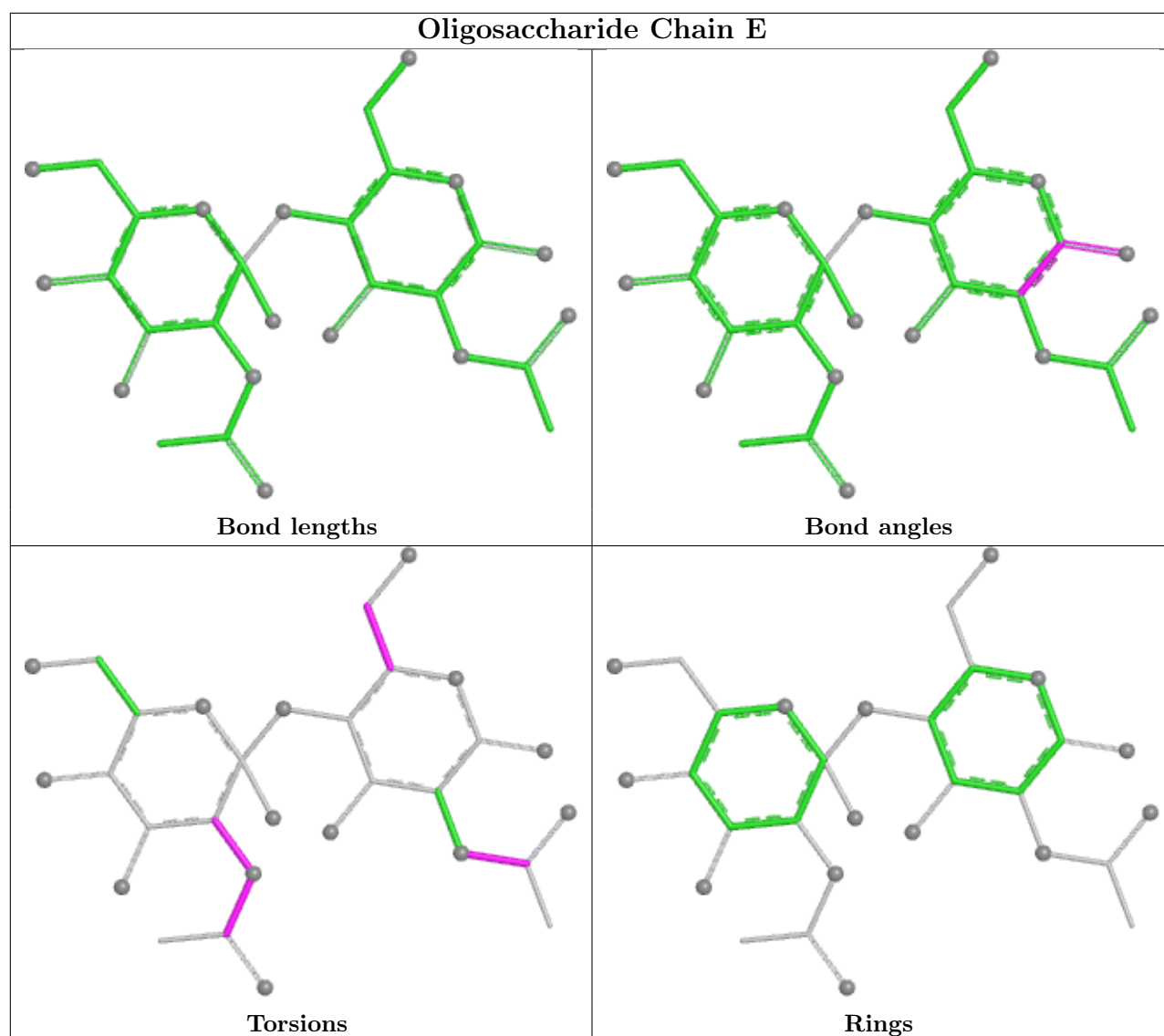
Mol	Chain	Res	Type	Atoms
2	H	1	NAG	C1-C2-N2-C7
2	H	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C3-C2-N2-C7

There are no ring outliers.

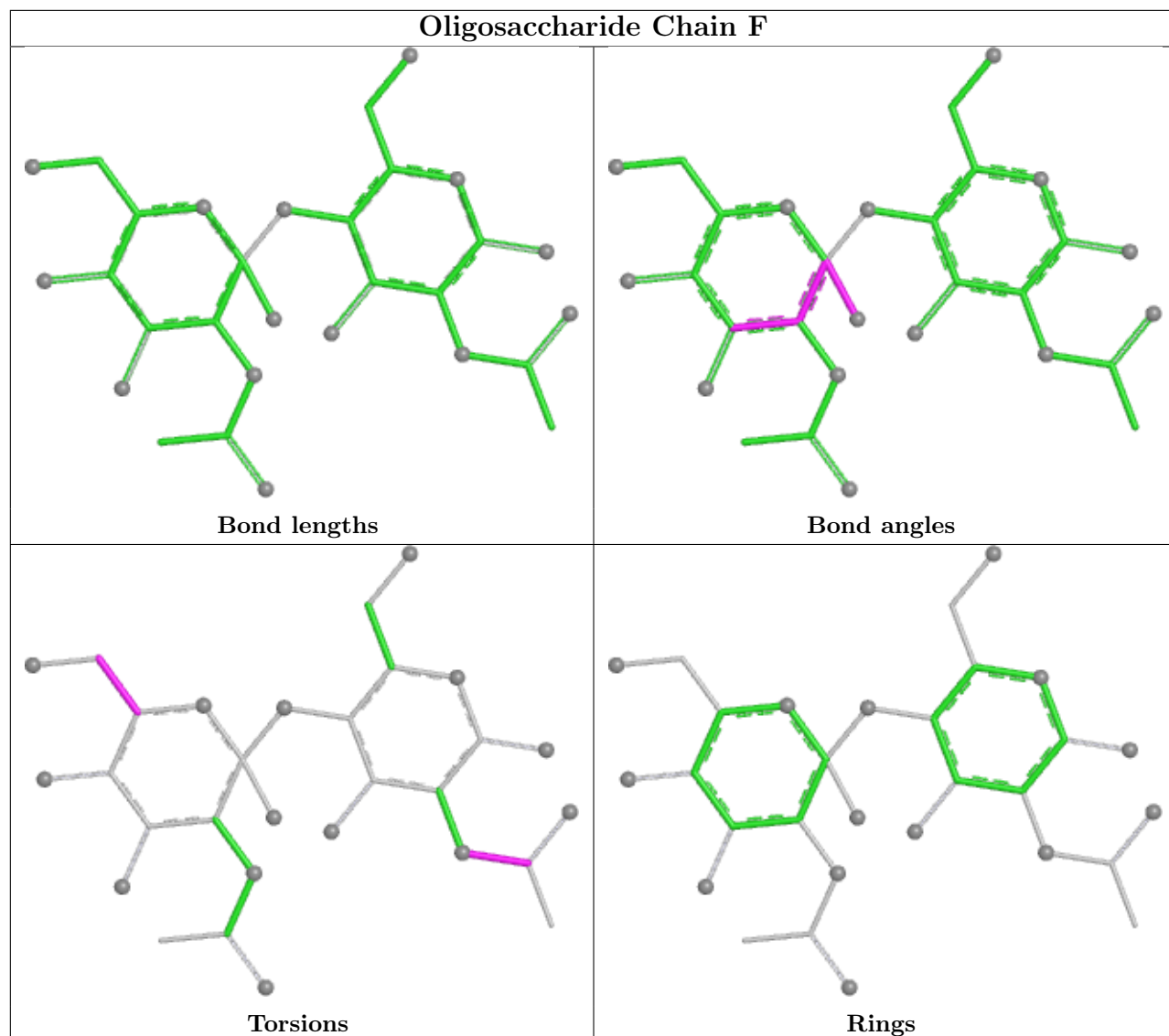
8 monomers are involved in 29 short contacts:

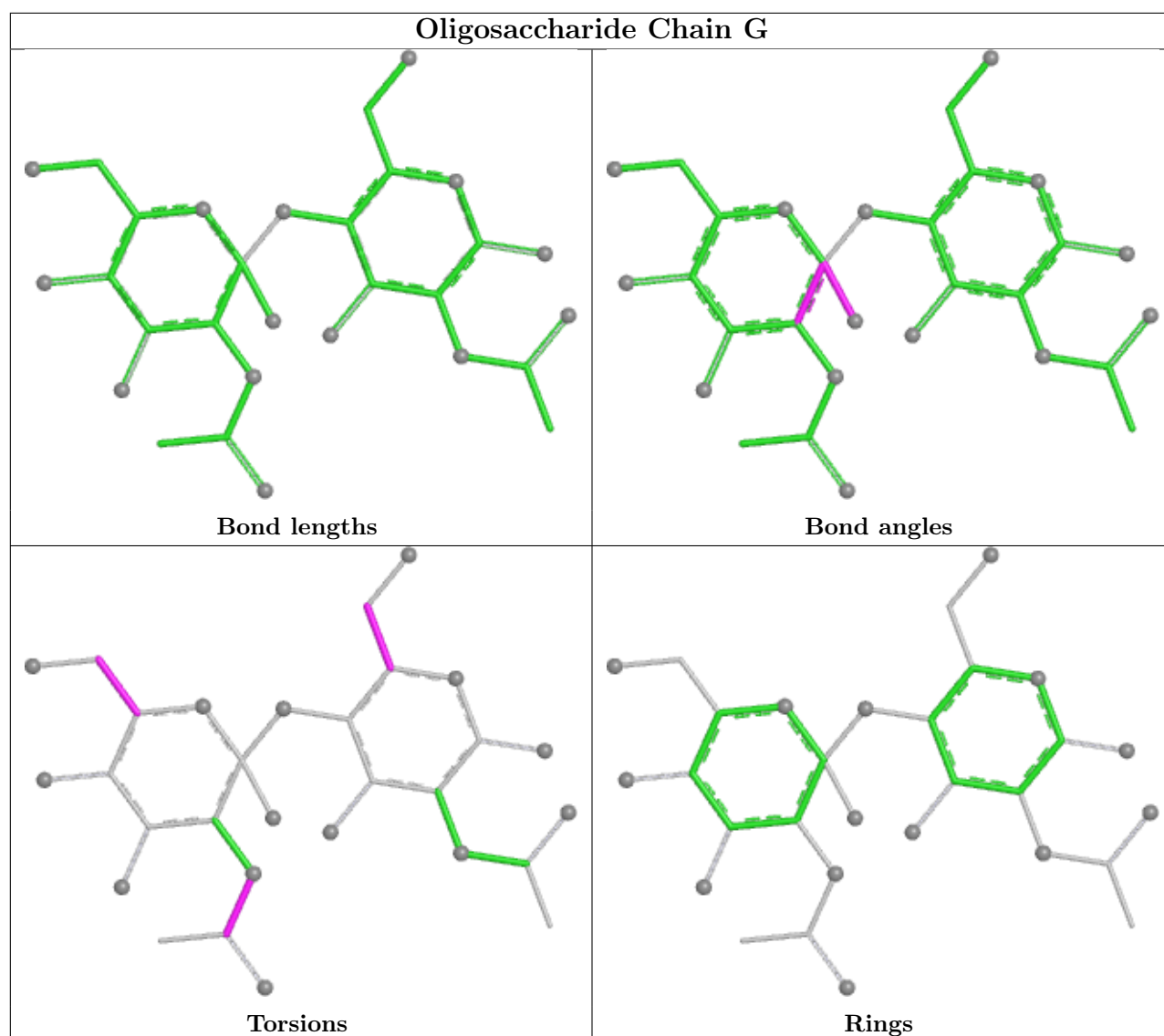
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	2	0
3	I	2	NAG	3	0
2	G	1	NAG	9	0
2	F	1	NAG	4	0
2	E	1	NAG	4	0
2	H	1	NAG	7	0
2	H	2	NAG	4	0
3	I	1	NAG	4	0

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

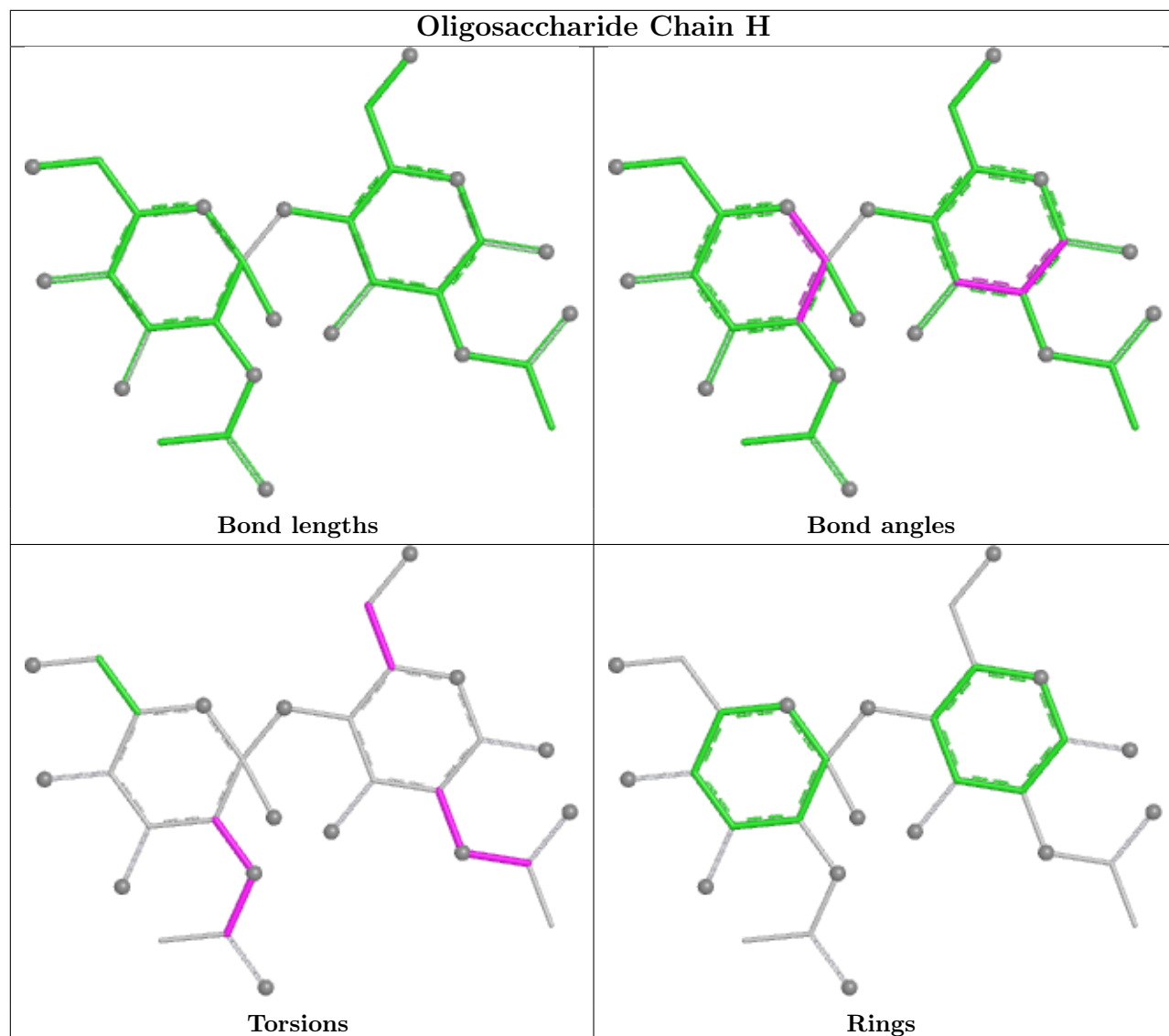


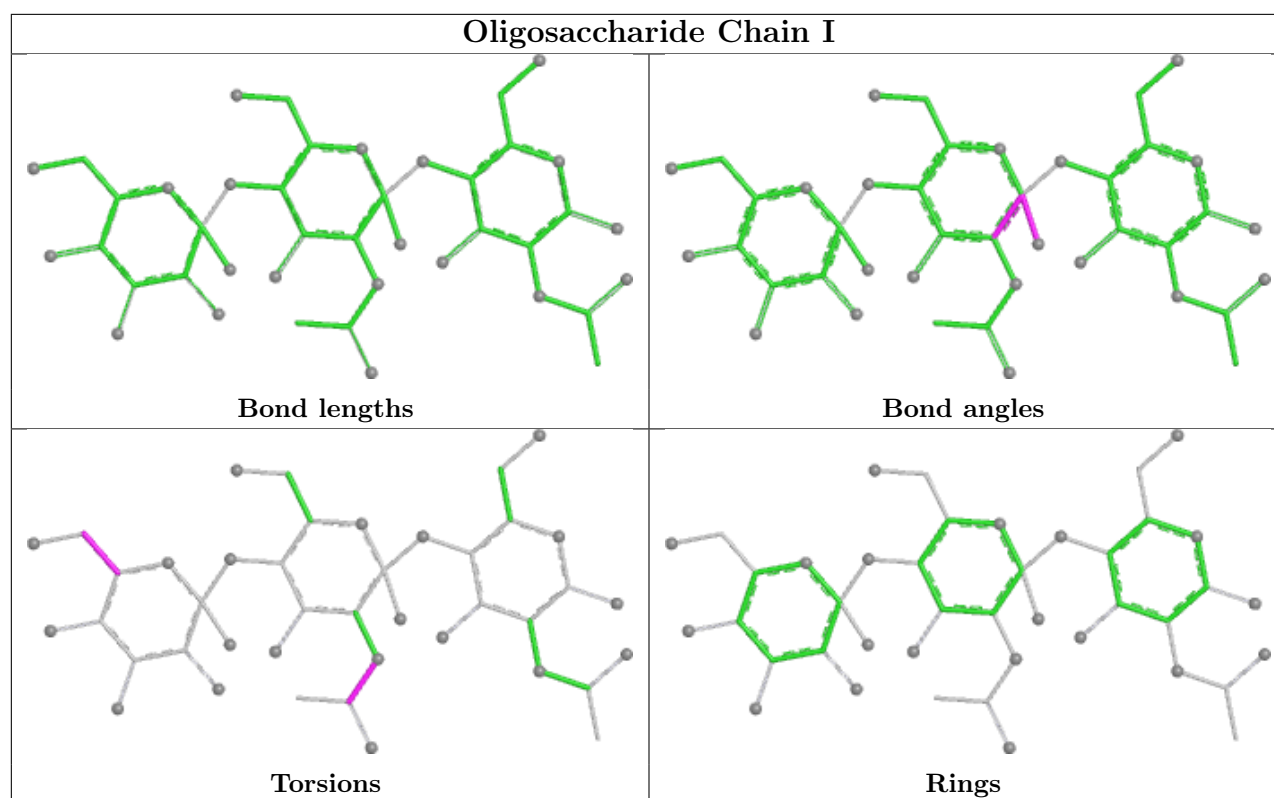
## Oligosaccharide Chain F





## Oligosaccharide Chain H





## 5.6 Ligand geometry [i](#)

14 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	1PE	B	1403	-	15,15,15	0.72	0	14,14,14	1.46	4 (28%)
4	2BF	D	3402	-	20,20,20	4.33	16 (80%)	24,27,27	1.26	3 (12%)
5	1PE	D	3403	-	15,15,15	0.84	0	14,14,14	1.46	4 (28%)
5	1PE	A	402	-	15,15,15	0.90	0	14,14,14	1.50	4 (28%)
4	2BF	B	1402	-	20,20,20	4.15	15 (75%)	24,27,27	1.35	3 (12%)
4	2BF	C	2401	-	20,20,20	4.20	15 (75%)	24,27,27	1.38	4 (16%)
5	1PE	A	403	-	15,15,15	0.79	0	14,14,14	1.53	4 (28%)
4	2BF	A	401	-	20,20,20	4.34	14 (70%)	24,27,27	1.32	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	1PE	C	2403	-	15,15,15	0.88	0	14,14,14	1.51	4 (28%)
6	NDG	B	1401	-	15,15,15	0.31	0	21,21,21	0.65	0
7	NAG	D	3401	1	15,15,15	0.43	0	21,21,21	0.62	0
5	1PE	A	404	-	15,15,15	0.95	0	14,14,14	1.51	4 (28%)
5	1PE	C	2402	-	15,15,15	0.86	0	14,14,14	1.52	4 (28%)
5	1PE	B	1404	-	15,15,15	0.83	0	14,14,14	1.52	4 (28%)

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	1PE	B	1403	-	-	5/13/13/13	-
4	2BF	D	3402	-	-	7/15/15/15	0/2/2/2
5	1PE	D	3403	-	-	3/13/13/13	-
5	1PE	A	402	-	-	8/13/13/13	-
4	2BF	B	1402	-	-	7/15/15/15	0/2/2/2
4	2BF	C	2401	-	-	1/15/15/15	0/2/2/2
5	1PE	A	403	-	-	6/13/13/13	-
4	2BF	A	401	-	-	7/15/15/15	0/2/2/2
5	1PE	C	2403	-	-	8/13/13/13	-
6	NDG	B	1401	-	-	4/6/26/26	0/1/1/1
7	NAG	D	3401	1	1/1/6/7	5/6/26/26	0/1/1/1
5	1PE	A	404	-	-	5/13/13/13	-
5	1PE	C	2402	-	-	4/13/13/13	-
5	1PE	B	1404	-	-	6/13/13/13	-

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	2BF	C9-C8	9.14	1.56	1.38
4	C	2401	2BF	C9-C8	9.08	1.56	1.38
4	D	3402	2BF	C9-C8	8.98	1.56	1.38
4	B	1402	2BF	C9-C8	8.95	1.56	1.38
4	A	401	2BF	C12-C11	7.88	1.55	1.38

The worst 5 of 45 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1402	2BF	O1P-P-C7	-4.26	104.03	110.89
4	C	2401	2BF	O1P-P-C7	-3.93	104.56	110.89
4	A	401	2BF	O1P-P-C7	-3.39	105.42	110.89
4	D	3402	2BF	C8-C19-N	-2.88	105.73	112.66
5	C	2403	1PE	C25-OH5-C14	2.74	125.26	113.26

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	D	3401	NAG	C1

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	2BF	C5-C7-P-O1P
4	A	401	2BF	C5-C7-P-O2P
4	A	401	2BF	C5-C7-P-O3P
4	A	401	2BF	N-C7-P-O1P
4	A	401	2BF	N-C7-P-O2P

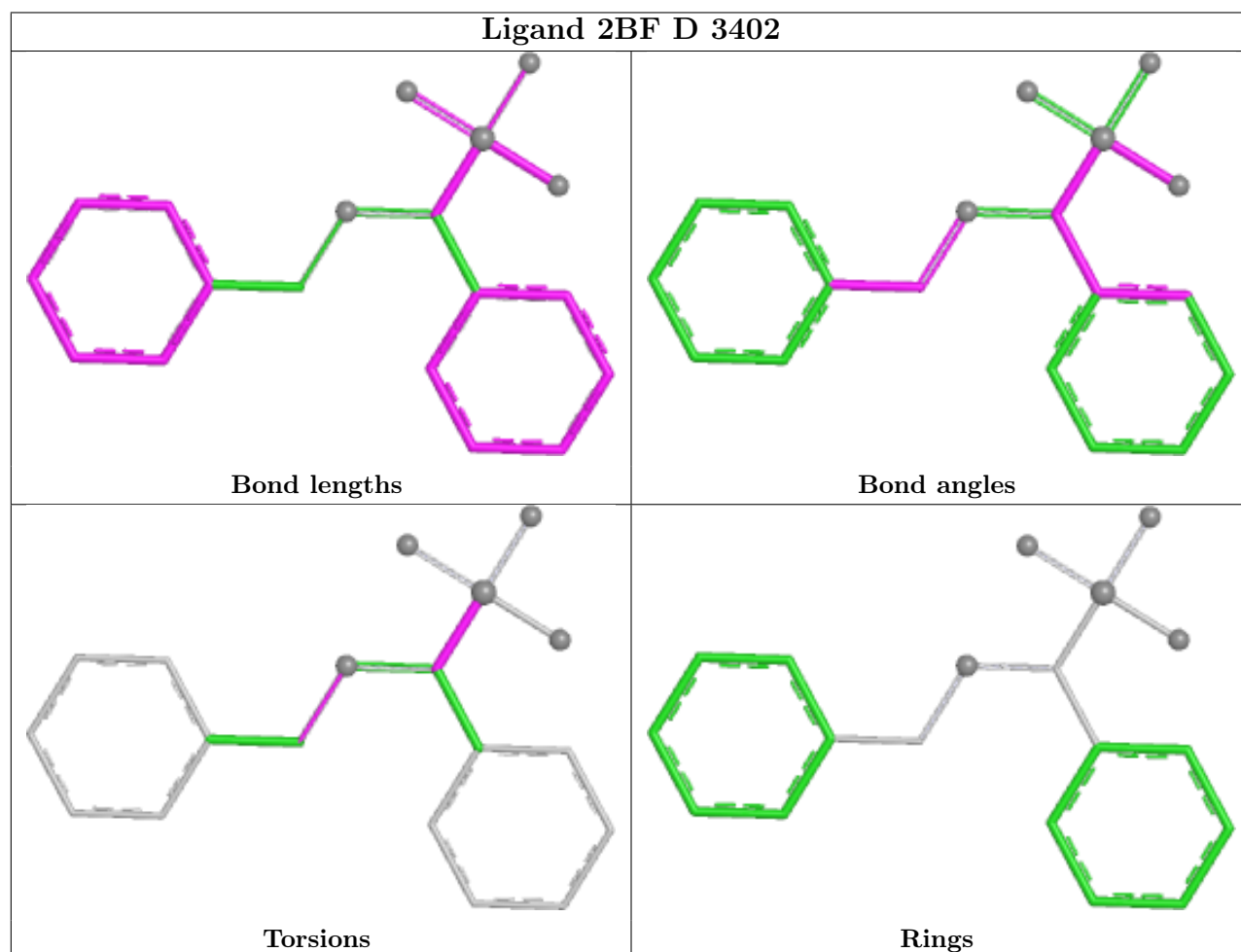
There are no ring outliers.

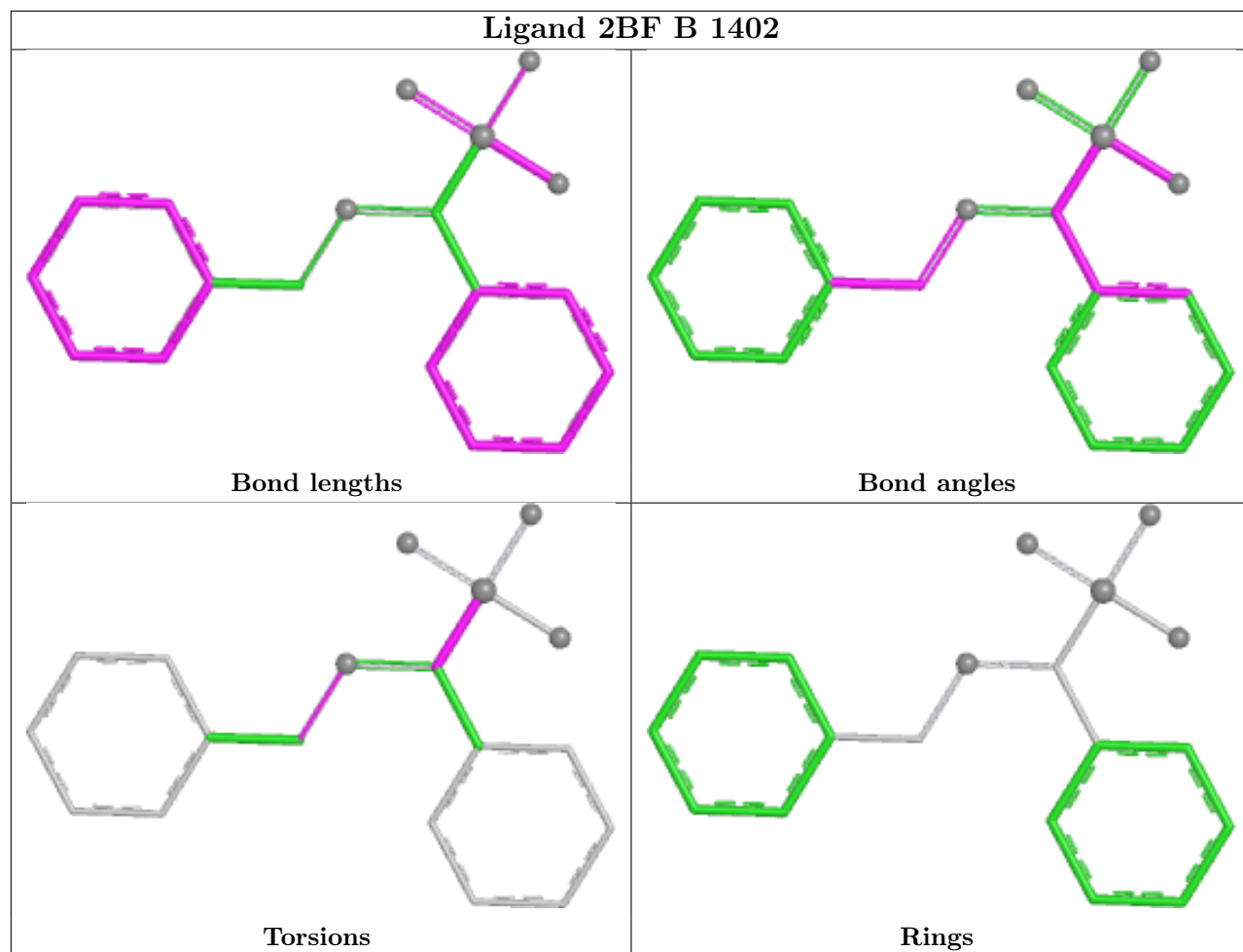
12 monomers are involved in 31 short contacts:

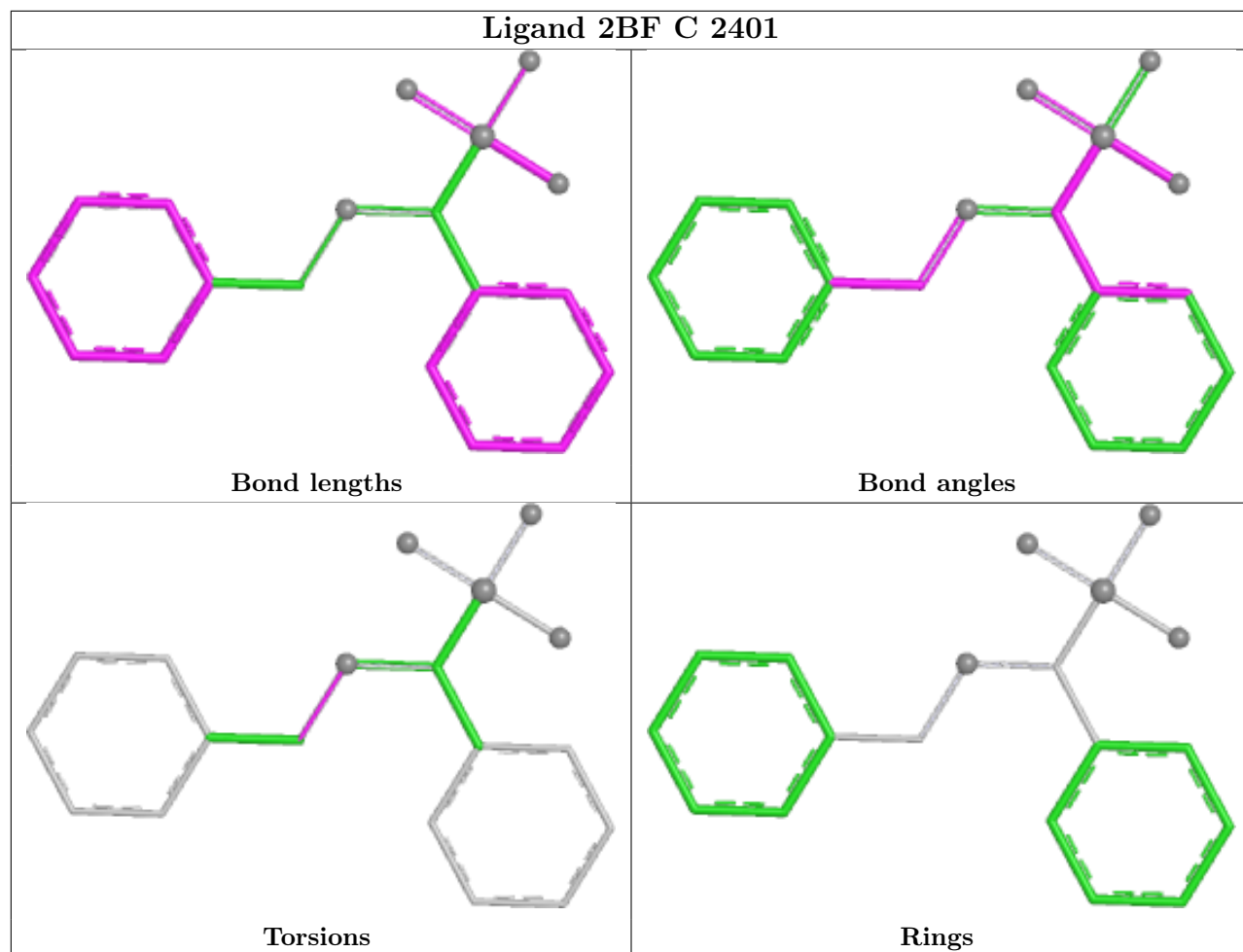
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1403	1PE	1	0
5	D	3403	1PE	1	0
5	A	402	1PE	1	0
4	B	1402	2BF	2	0
4	C	2401	2BF	2	0
5	A	403	1PE	2	0
4	A	401	2BF	3	0
5	C	2403	1PE	1	0
6	B	1401	NDG	7	0
7	D	3401	NAG	6	0
5	C	2402	1PE	1	0
5	B	1404	1PE	4	0

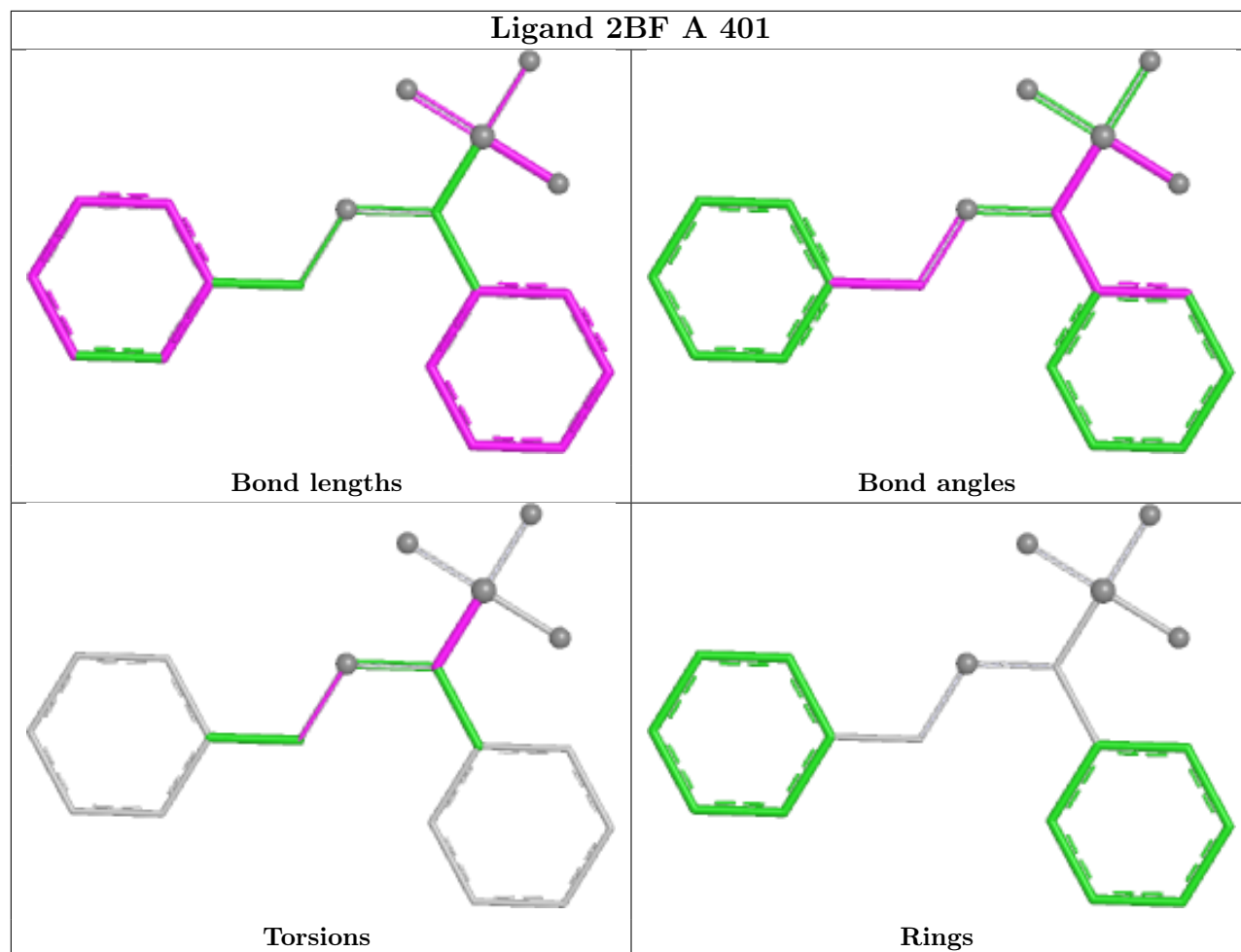
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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