WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 29, 2024 – 01:56 AM EDT

PDB ID	:	1HZX
Title	:	CRYSTAL STRUCTURE OF BOVINE RHODOPSIN
Authors	:	Teller, D.C.; Okada, T.; Behnke, C.A.; Palczewski, K.; Stenkamp, R.E.
Deposited on	:	2001-01-26
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 (i) 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 (i)) were used in the production of this report:

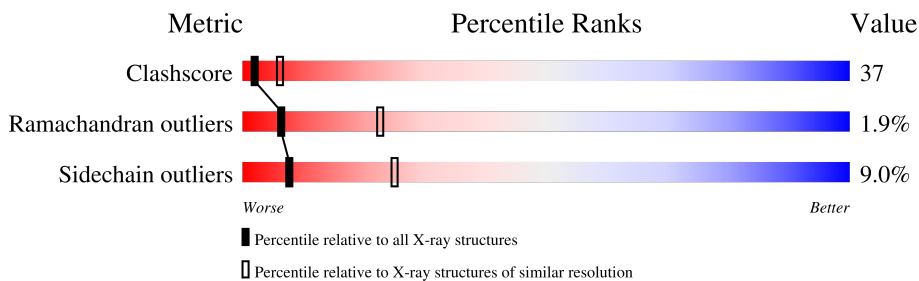|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Clashscore		37
Ramachandran outliers		1.9%
Sidechain outliers		9.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	349	42% 47% 8% ••
1	B	349	39% 42% 6% 13%
2	C	3	33% 67%
3	D	2	50% 50%
3	F	2	100%
4	E	4	50% 25% 25%

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 crite-

ria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BNG	B	1506	-	-	X	-

2   Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 5551 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 RHODOPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total 2685	C 1783	N 413	O 463	S 26	0	0	0
1	B	302	Total 2398	C 1603	N 366	O 404	S 25	0	0	0

- Molecule 2 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.
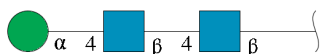
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total 39	C 22	N 2	O 15	0	0	0

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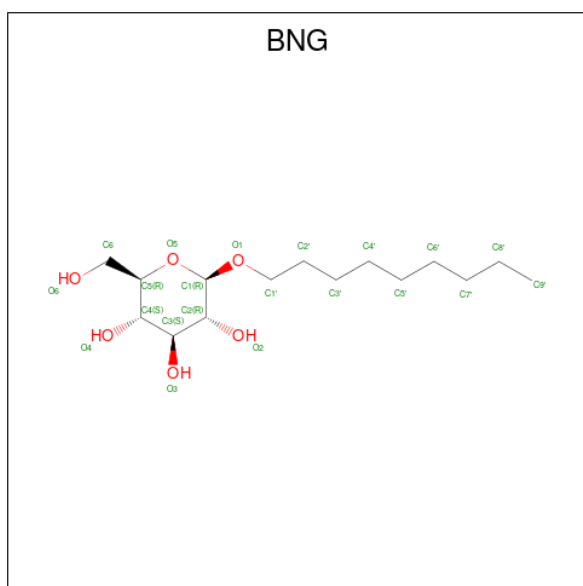

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total 28	C 16	N 2	O 10	0	0	0
3	F	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-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
4	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			21	15	6		
5	A	1	Total	C	O	0	0
			21	15	6		
5	A	1	Total	C	O	0	0
			21	15	6		
5	A	1	Total	C	O	0	0
			21	15	6		
5	A	1	Total	C	O	0	0
			21	15	6		
5	B	1	Total	C	O	0	0
			21	15	6		
5	B	1	Total	C	O	0	0
			21	15	6		

- Molecule 6 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	Hg 3	0	0
6	B	3	Total 3	Hg 3	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total 4	Zn 4	0	0
7	B	3	Total 3	Zn 3	0	0

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).
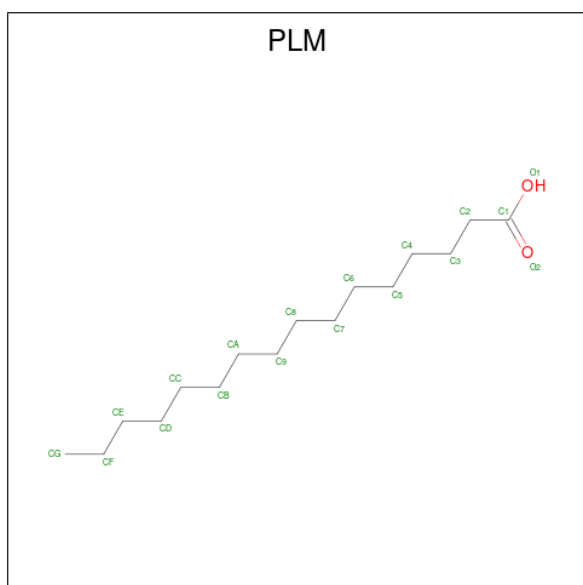
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 17	C 16	O 1	0	0
8	A	1	Total 17	C 16	O 1	0	0
8	B	1	Total 17	C 16	O 1	0	0

- Molecule 9 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).

RET
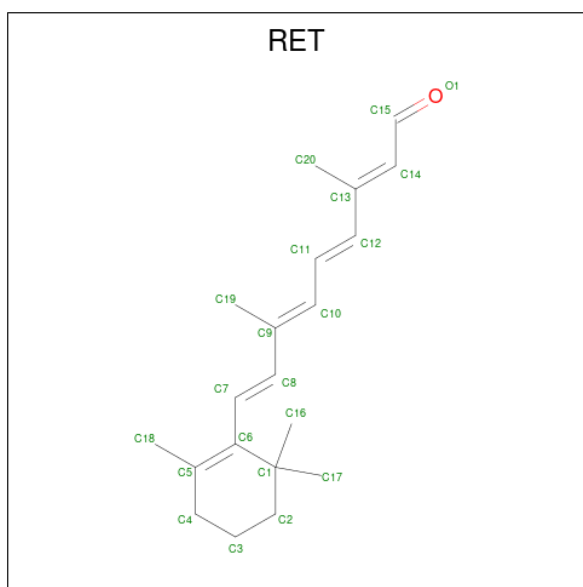
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total 20	C 20	0	0
9	B	1	Total 20	C 20	0	0

• Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).

HTO

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total 10	C 7	O 3	0	0
10	A	1	Total 10	C 7	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total 10	C 7	O 3	0	0
10	A	1	Total 10	C 7	O 3	0	0
10	B	1	Total 10	C 7	O 3	0	0
10	B	1	Total 10	C 7	O 3	0	0

- Molecule 11 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	7	Total 7	O 7	0	0
11	B	5	Total 5	O 5	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.
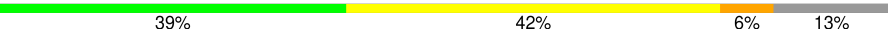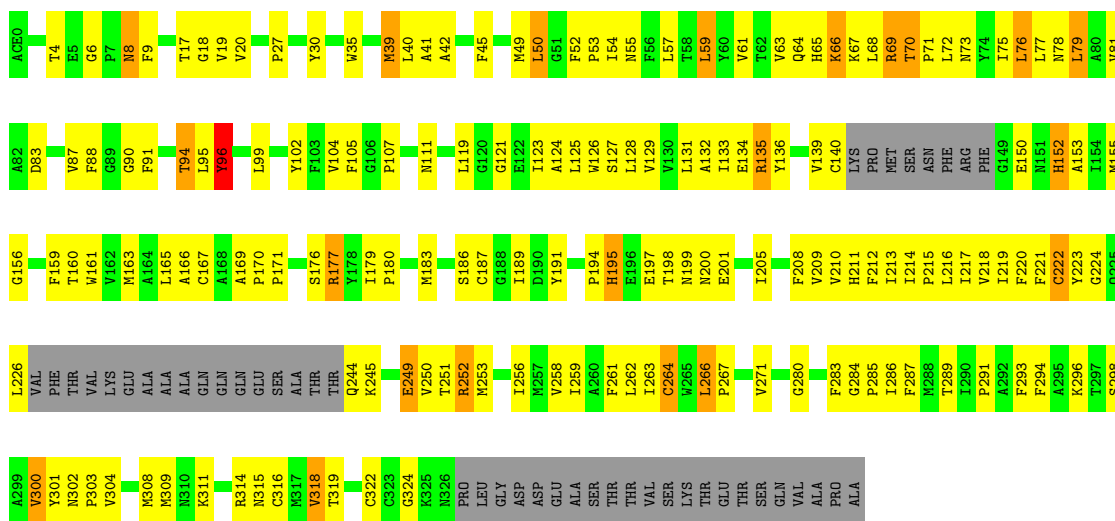
Note EDS was not executed.

• Molecule 1: RHODOPSIN

Chain A:
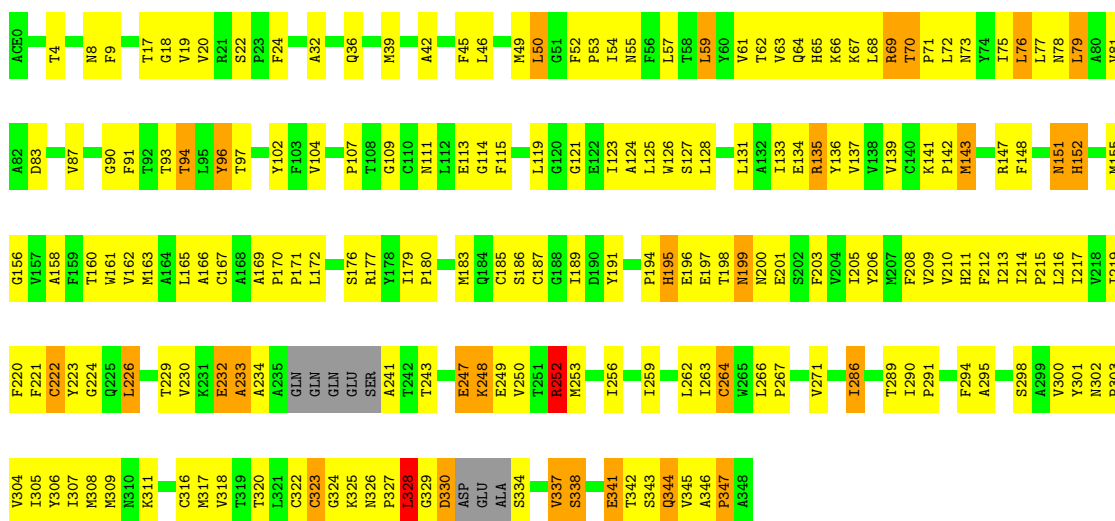
• Molecule 1: RHODOPSIN

Chain B:

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

Chain C:

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

Chain D:

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

Chain F:

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

Chain E:

4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	97.25Å　97.25Å　149.54Å 90.00°　90.00°　90.00°	Depositor
Resolution (Å)	30.00　–　2.80	Depositor
% Data completeness (in resolution range)	69.8 (30.00-2.80)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program		Depositor
R, R_{free}	0.175　,　0.212	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5551	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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: HG, PLM, MAN, BMA, NAG, BNG, ZN, ACE, HTO, RET

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	0.53	2/2765 (0.1%)	0.74	2/3767 (0.1%)
1	B	0.53	2/2472 (0.1%)	0.72	1/3368 (0.0%)
All	All	0.53	4/5237 (0.1%)	0.73	3/7135 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	TYR	CB-CG	-5.68	1.43	1.51
1	A	96	TYR	CB-CG	-5.49	1.43	1.51
1	B	249	GLU	CD-OE1	-5.28	1.19	1.25
1	A	249	GLU	CD-OE1	-5.18	1.20	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	177	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	B	177	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	A	252	ARG	NE-CZ-NH2	5.24	122.92	120.30

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	2685	0	2655	232	1
1	B	2398	0	2368	198	0
2	C	39	0	34	5	0
3	D	28	0	25	2	0
3	F	28	0	25	1	0
4	E	50	0	43	2	0
5	A	105	0	150	10	0
5	B	42	0	60	10	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	4	0	0	0	0
7	B	3	0	0	0	1
8	A	34	0	62	1	0
8	B	17	0	31	1	0
9	A	20	0	27	1	0
9	B	20	0	27	1	0
10	A	40	0	64	5	0
10	B	20	0	32	2	0
11	A	7	0	0	0	0
11	B	5	0	0	1	0
All	All	5551	0	5603	415	1

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 37.

The worst 5 of 415 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:328:LEU:HB2	1:B:96:TYR:CE2	1.67	1.29
1:A:50:LEU:HD12	1:B:50:LEU:HD12	1.11	1.09
1:A:50:LEU:HD12	1:B:50:LEU:CD1	1.83	1.09
1:A:65:HIS:HB3	1:A:337:VAL:HG22	1.38	1.06
1:A:328:LEU:HB2	1:B:96:TYR:HE2	1.04	1.02

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLU:OE2	7:B:958:ZN:ZN[2_654]	1.56	0.64

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	335/349 (96%)	275 (82%)	50 (15%)	10 (3%)	3	13
1	B	296/349 (85%)	256 (86%)	38 (13%)	2 (1%)	19	48
All	All	631/698 (90%)	531 (84%)	88 (14%)	12 (2%)	6	23

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ALA
1	A	328	LEU
1	A	341	GLU
1	A	195	HIS
1	A	232	GLU

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	289/296 (98%)	262 (91%)	27 (9%)	7	23
1	B	257/296 (87%)	235 (91%)	22 (9%)	8	27
All	All	546/592 (92%)	497 (91%)	49 (9%)	8	25

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	27	PRO

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Mol	Chain	Res	Type
1	B	76	LEU
1	B	39	MET
1	B	66	LYS
1	B	94	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	111	ASN
1	B	199	ASN
1	B	315	ASN
1	B	302	ASN
1	A	302	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	C	1	2,1	14,14,15	0.66	0	17,19,21	0.72	0
2	NAG	C	2	2	14,14,15	0.66	0	17,19,21	0.97	0
2	MAN	C	3	2	11,11,12	0.69	0	15,15,17	0.69	0
3	NAG	D	1	3,1	14,14,15	0.55	0	17,19,21	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
3	NAG	D	2	3	14,14,15	0.83	0	17,19,21	0.88	0
4	NAG	E	1	4,1	14,14,15	0.46	0	17,19,21	0.84	0
4	NAG	E	2	4	14,14,15	0.51	0	17,19,21	0.87	1 (5%)
4	BMA	E	3	4	11,11,12	0.74	0	15,15,17	0.53	0
4	BMA	E	4	4	11,11,12	0.68	0	15,15,17	0.63	0
3	NAG	F	1	3,1	14,14,15	0.66	0	17,19,21	0.75	0
3	NAG	F	2	3	14,14,15	0.81	1 (7%)	17,19,21	0.66	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	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	MAN	C	3	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	5/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	4/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	BMA	E	4	4	-	2/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	C1-C2	2.08	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	2	NAG	C2-N2-C7	-2.58	119.45	122.90
3	D	1	NAG	C2-N2-C7	-2.11	120.07	122.90

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
3	D	1	NAG	C8-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	3	0
3	F	1	NAG	1	0
3	D	2	NAG	2	0
4	E	1	NAG	2	0
4	E	2	NAG	1	0
2	C	1	NAG	5	0
3	D	1	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 oligosaccharide.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings
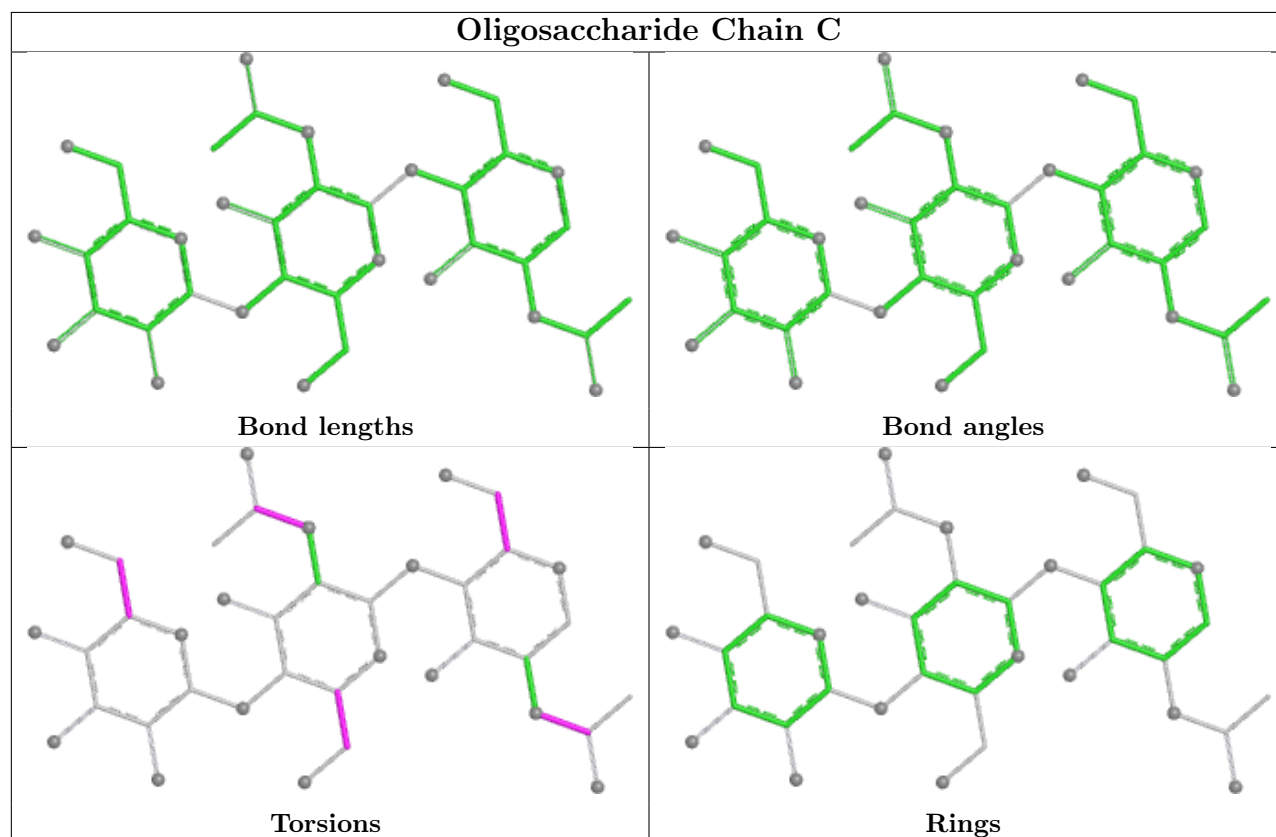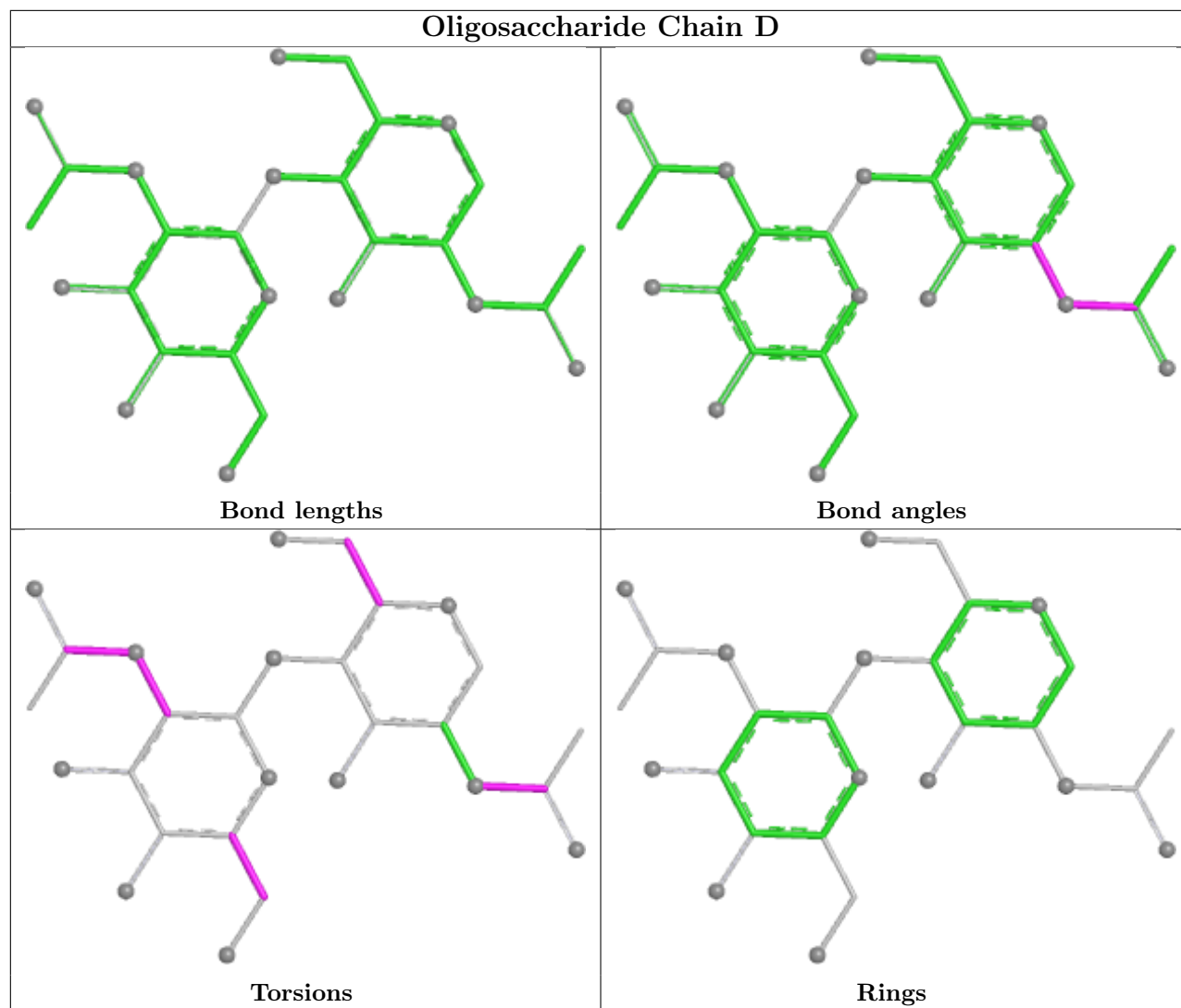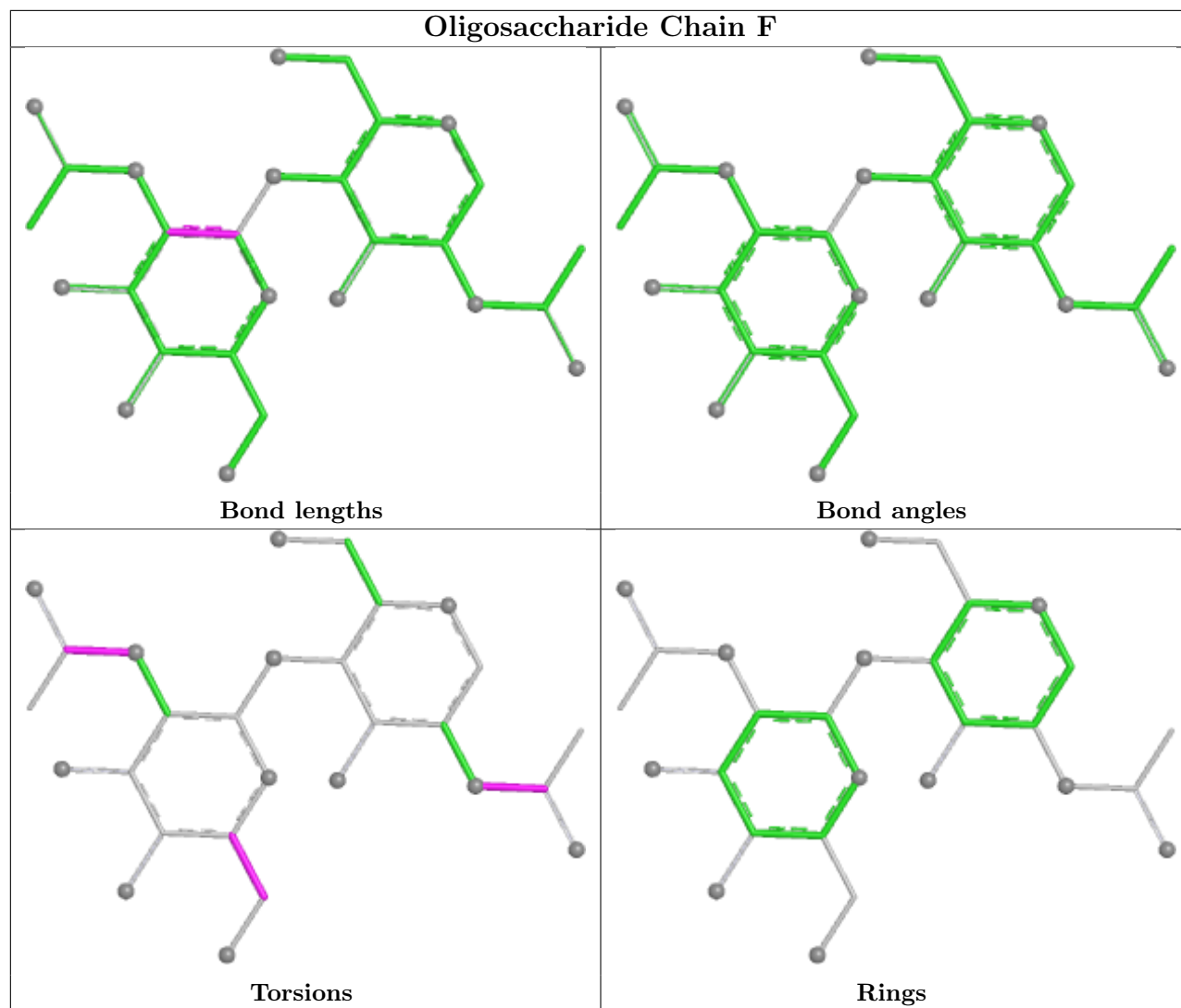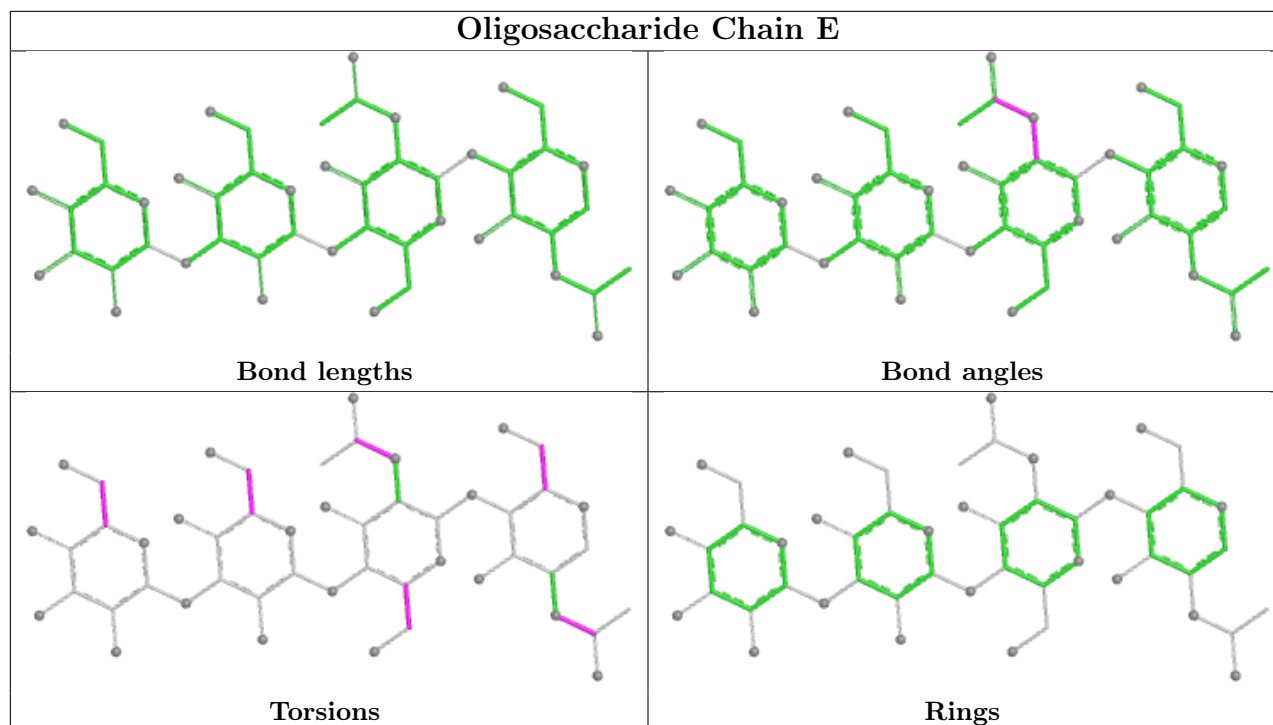
5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 13 are monoatomic - leaving 18 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	#$|Z| > 2$
5	BNG	B	1502	-	21,21,21	1.43	3 (14%)	26,26,26	0.64	0
10	HTO	A	1404	-	9,9,9	1.72	2 (22%)	10,10,10	0.70	0
5	BNG	A	1505	-	21,21,21	1.40	4 (19%)	26,26,26	0.66	0
8	PLM	A	1323	1	15,16,17	0.35	0	14,15,17	0.50	0
5	BNG	B	1506	-	21,21,21	1.37	3 (14%)	26,26,26	0.64	0
10	HTO	A	1400	-	9,9,9	1.71	2 (22%)	10,10,10	0.66	0
10	HTO	A	1405	-	9,9,9	1.37	1 (11%)	10,10,10	0.45	0
8	PLM	A	1322	1	15,16,17	0.21	0	14,15,17	0.59	0
8	PLM	B	1322	1	15,16,17	0.34	0	14,15,17	0.52	0
9	RET	A	1296	1	20,20,21	2.00	6 (30%)	27,27,28	1.95	10 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
10	HTO	A	1403	-	9,9,9	1.58	1 (11%)	10,10,10	0.50	0
5	BNG	A	1501	-	21,21,21	1.26	2 (9%)	26,26,26	0.65	0
10	HTO	B	1406	-	9,9,9	1.71	2 (22%)	10,10,10	0.78	0
5	BNG	A	1500	-	21,21,21	1.29	3 (14%)	26,26,26	0.60	0
5	BNG	A	1503	-	21,21,21	1.23	3 (14%)	26,26,26	0.60	0
9	RET	B	1296	1	20,20,21	1.95	6 (30%)	27,27,28	2.00	9 (33%)
10	HTO	B	1401	-	9,9,9	1.61	1 (11%)	10,10,10	0.81	0
5	BNG	A	1504	-	21,21,21	1.31	3 (14%)	26,26,26	0.60	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
5	BNG	B	1502	-	-	7/12/32/32	0/1/1/1
10	HTO	A	1404	-	-	4/10/10/10	-
5	BNG	A	1505	-	-	6/12/32/32	0/1/1/1
8	PLM	A	1323	1	-	8/14/14/15	-
5	BNG	B	1506	-	-	10/12/32/32	0/1/1/1
10	HTO	A	1400	-	-	3/10/10/10	-
10	HTO	A	1405	-	-	3/10/10/10	-
8	PLM	A	1322	1	-	10/14/14/15	-
8	PLM	B	1322	1	-	10/14/14/15	-
9	RET	A	1296	1	-	7/13/30/31	0/1/1/1
10	HTO	A	1403	-	-	3/10/10/10	-
5	BNG	A	1501	-	-	6/12/32/32	0/1/1/1
10	HTO	B	1406	-	-	3/10/10/10	-
5	BNG	A	1500	-	-	8/12/32/32	0/1/1/1
5	BNG	A	1503	-	-	7/12/32/32	0/1/1/1
9	RET	B	1296	1	-	5/13/30/31	0/1/1/1
10	HTO	B	1401	-	-	2/10/10/10	-
5	BNG	A	1504	-	-	8/12/32/32	0/1/1/1

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1296	RET	C14-C13	5.46	1.37	1.33
9	A	1296	RET	C14-C13	4.48	1.36	1.33
10	B	1401	HTO	C3-C2	4.02	1.62	1.53
10	A	1404	HTO	C3-C2	3.97	1.62	1.53
5	B	1502	BNG	O1-C1	3.97	1.46	1.40

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1296	RET	C11-C12-C13	4.81	139.56	126.36
9	B	1296	RET	C11-C12-C13	4.76	139.42	126.36
9	A	1296	RET	C17-C1-C6	3.95	116.44	110.24
9	B	1296	RET	C2-C1-C6	3.84	116.02	110.44
9	B	1296	RET	C19-C9-C8	-3.45	112.82	118.09

There are no chirality outliers.

5 of 110 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1506	BNG	C2'-C1'-O1-C1
8	A	1323	PLM	C1-C2-C3-C4
8	B	1322	PLM	O2-C1-C2-C3
9	A	1296	RET	C20-C13-C14-C15
9	B	1296	RET	C11-C12-C13-C14

There are no ring outliers.
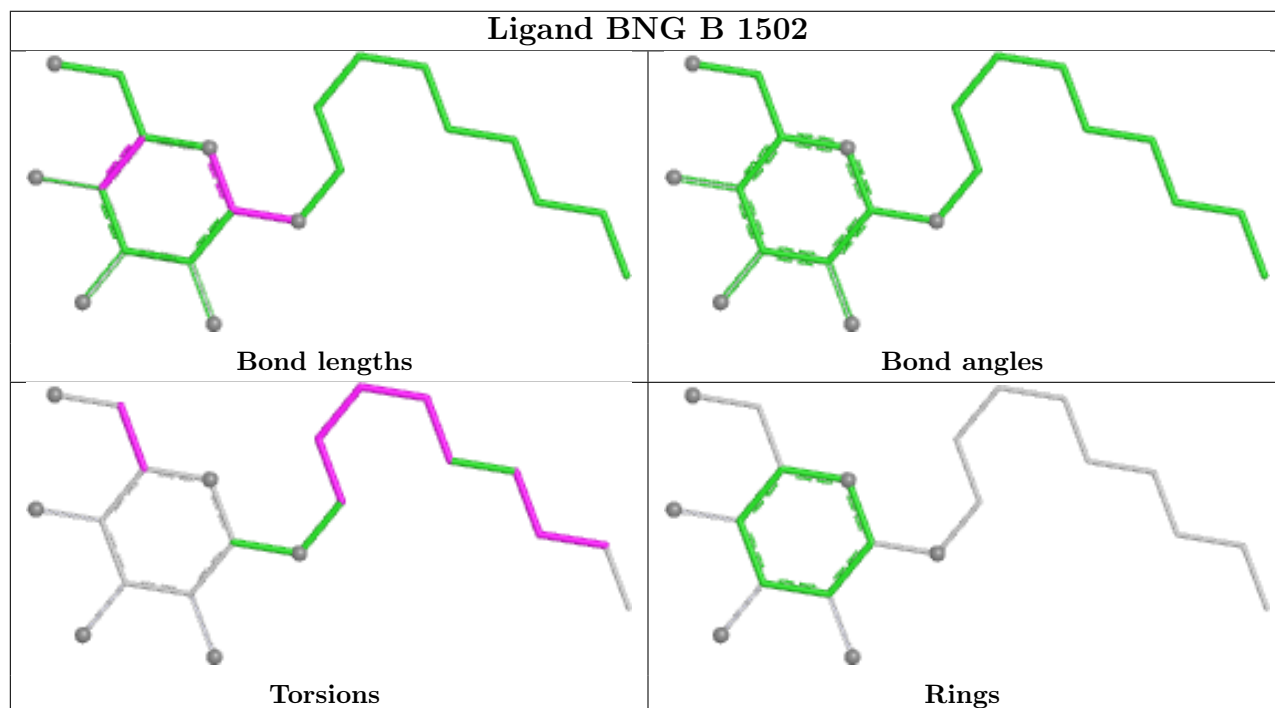
15 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1404	HTO	2	0
5	A	1505	BNG	1	0
5	B	1506	BNG	10	0
10	A	1400	HTO	1	0
8	A	1322	PLM	1	0
8	B	1322	PLM	1	0
9	A	1296	RET	1	0
10	A	1403	HTO	2	0
5	A	1501	BNG	2	0
10	B	1406	HTO	1	0
5	A	1500	BNG	5	0
5	A	1503	BNG	1	0
9	B	1296	RET	1	0

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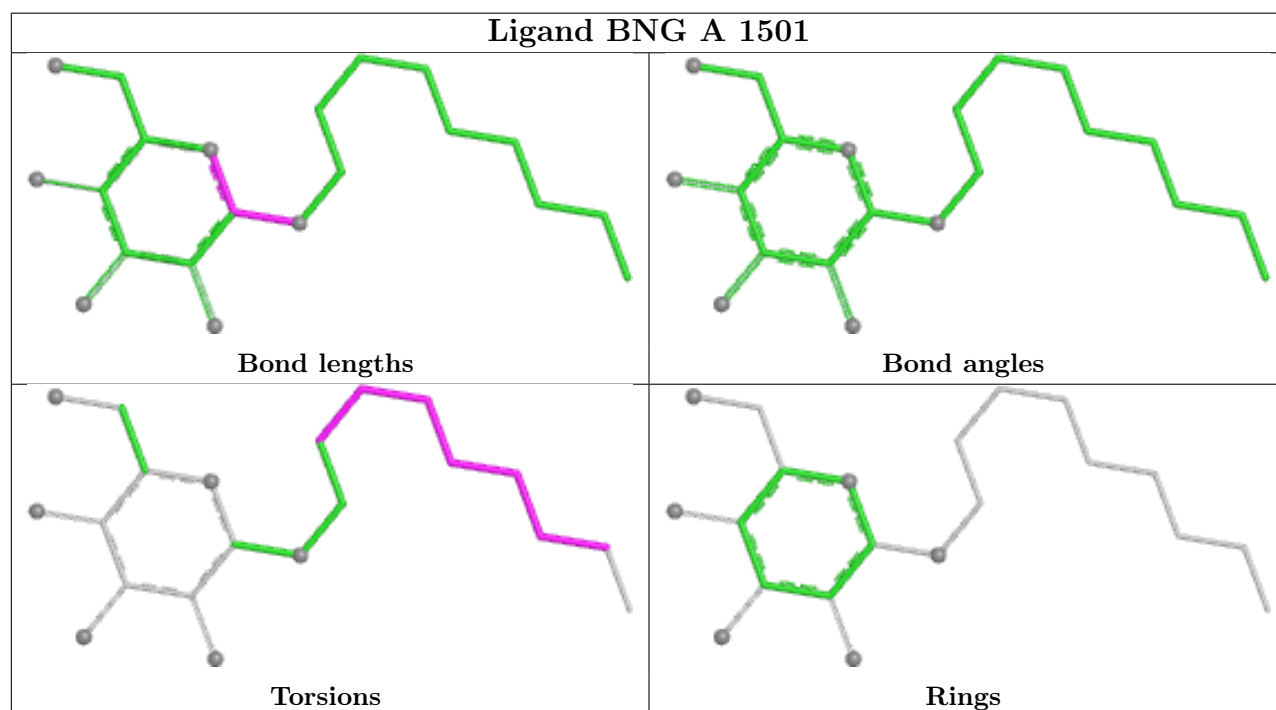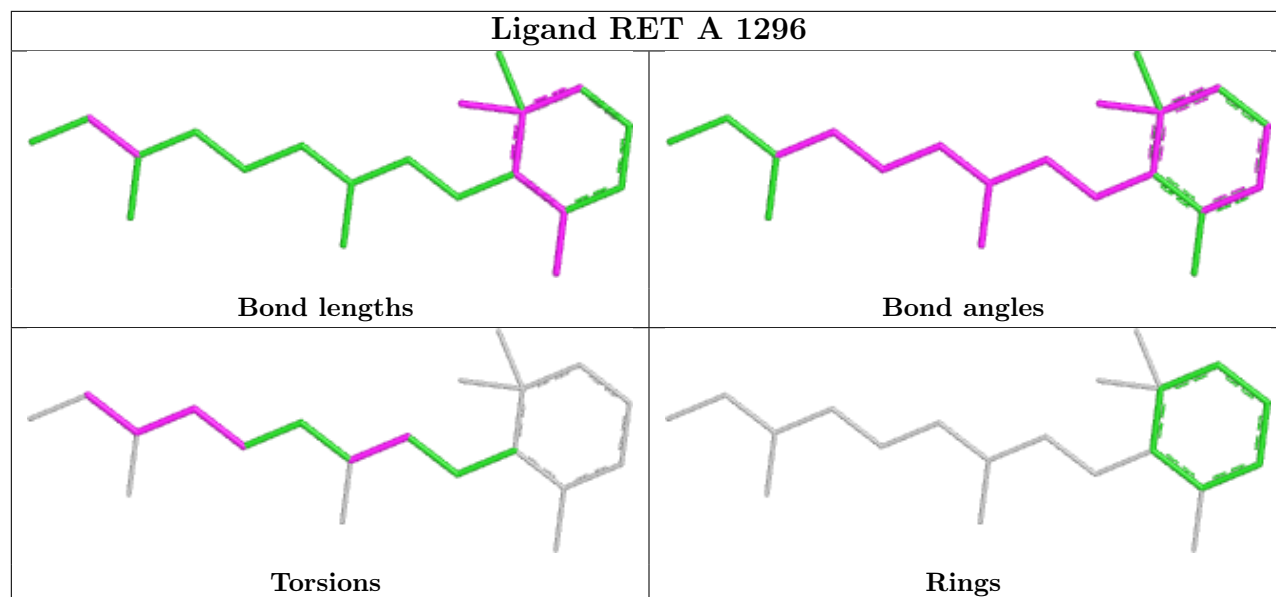| Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1401	HTO	1	0
5	A	1504	BNG	1	0

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 then 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.
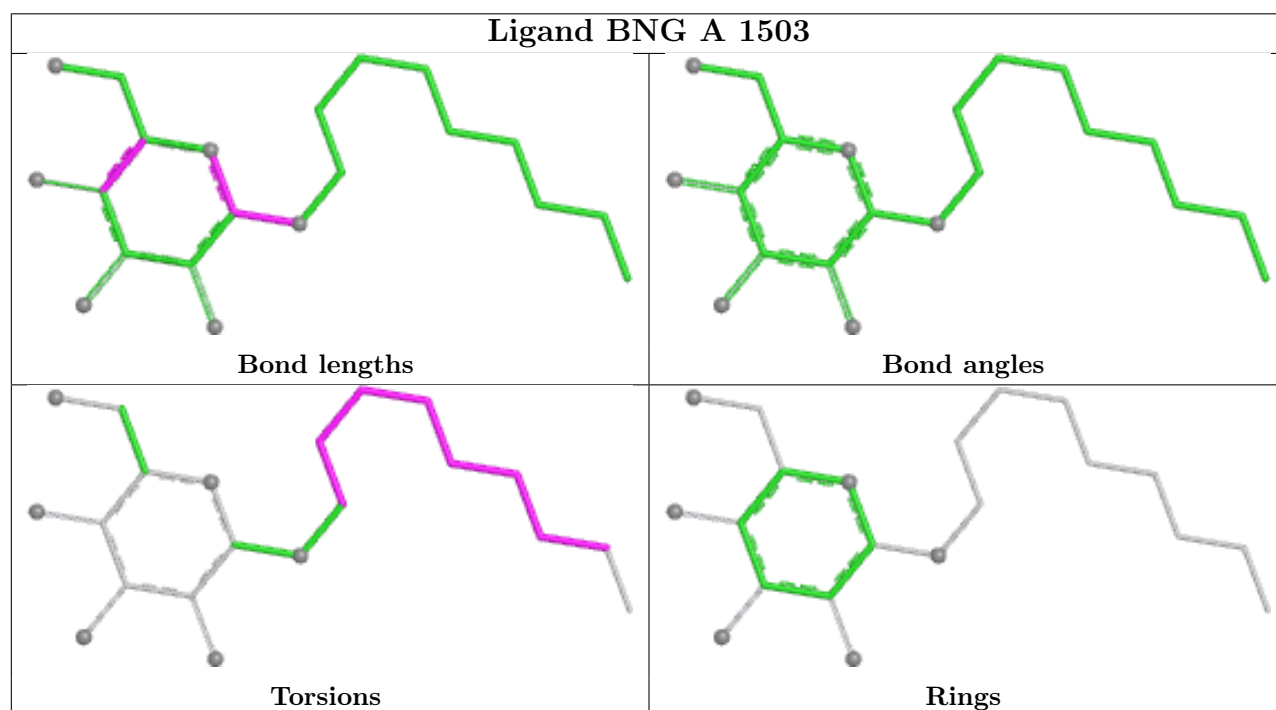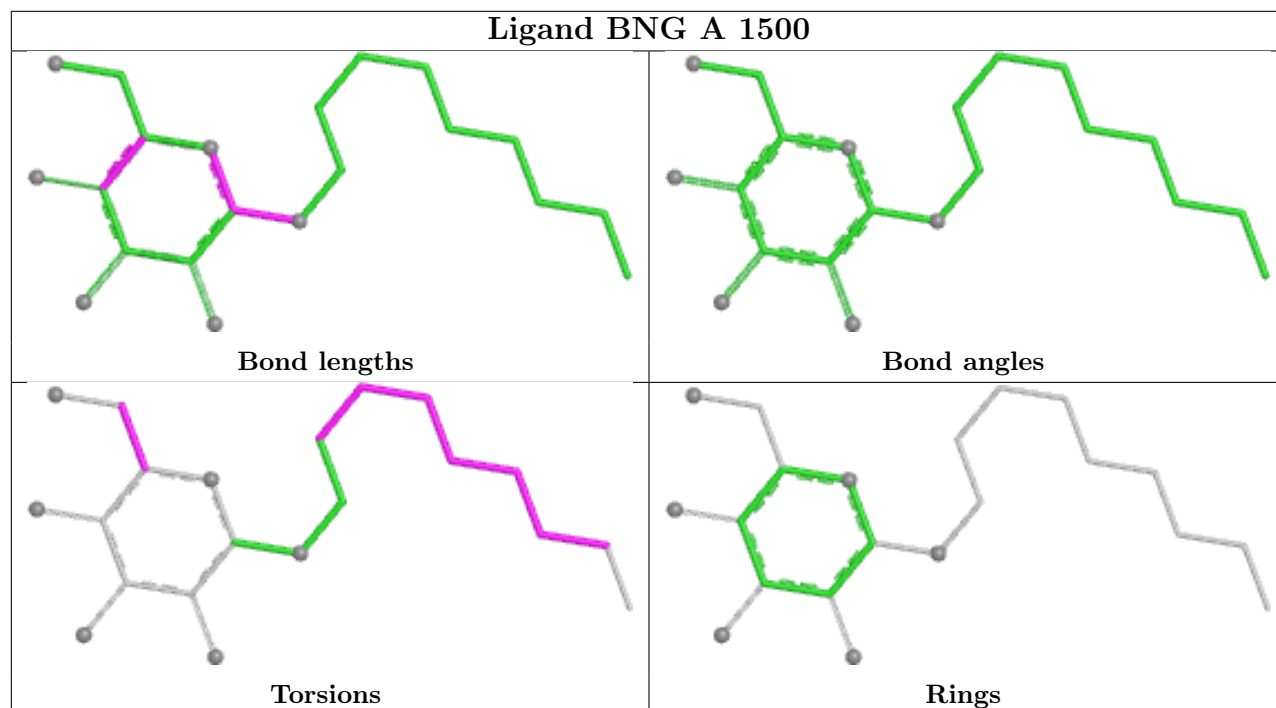

Ligand BNG B 1502

Bond lengths

Bond angles

Torsions

Rings

Ligand BNG A 1505

Bond lengths

Bond angles

Torsions

Rings

Ligand PLM A 1323

Bond lengths

Bond angles

Torsions

Rings

Ligand BNG B 1506

Bond lengths

Bond angles

Torsions

Rings

Ligand PLM A 1322

Bond lengths

Bond angles

Torsions

Rings

Ligand PLM B 1322

Bond lengths

Bond angles

Torsions

Rings

Ligand RET A 1296

Bond lengths

Bond angles

Torsions

Rings

Ligand BNG A 1501

Bond lengths

Bond angles

Torsions

Rings

Ligand BNG A 1500

Bond lengths

Bond angles

Torsions

Rings

Ligand BNG A 1503

Bond lengths

Bond angles

Torsions

Rings

Ligand RET B 1296

Bond lengths

Bond angles

Torsions

Rings

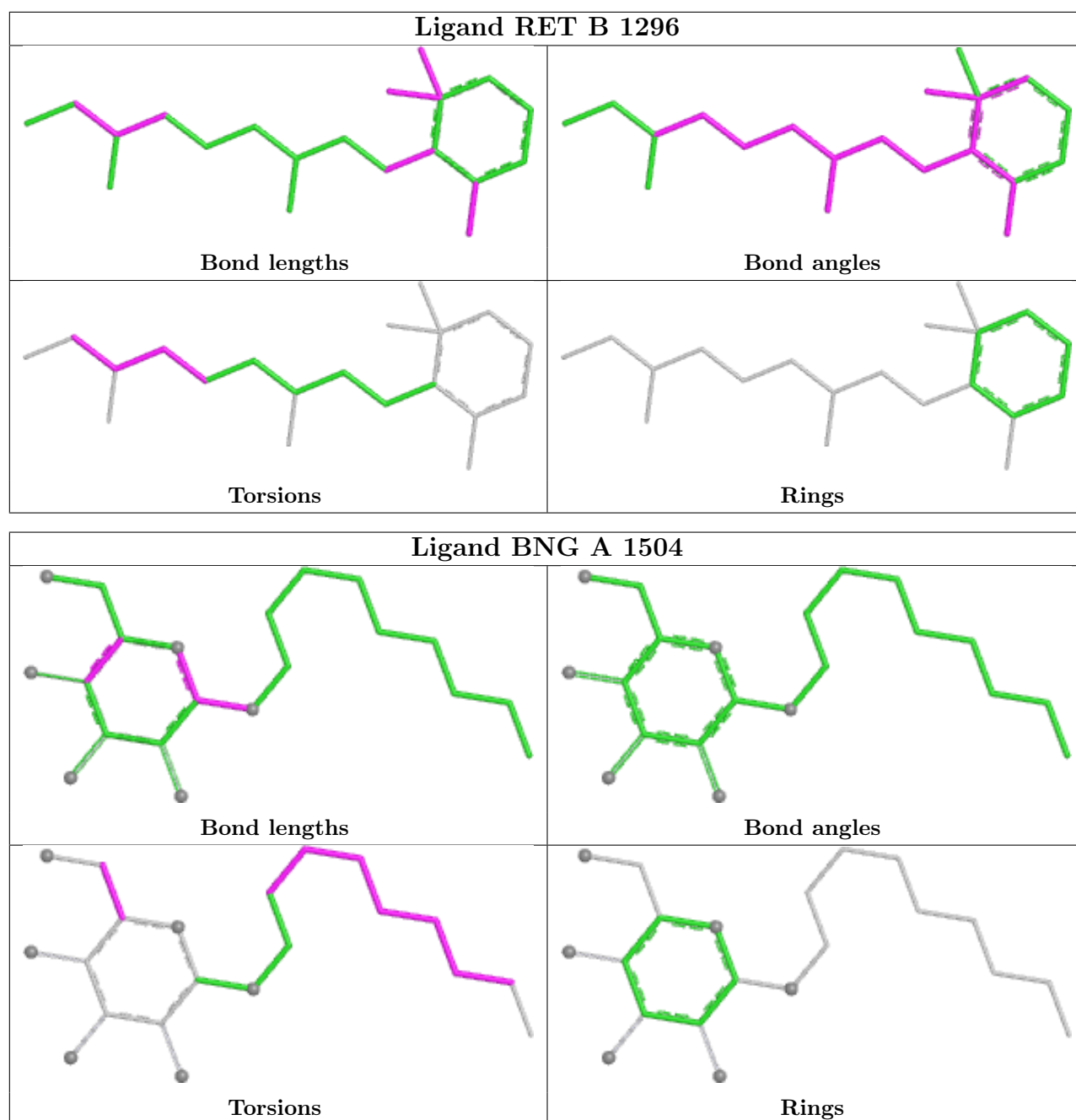**Ligand BNG A 1504**

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.