



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:52 AM UTC

PDB ID : 8P1G / pdb_00008p1g
Title : Crystal structure of inactive TtCE16 in complex with acetate
Authors : Dimarogona, M.; Kosinas, C.; Pentari, C.; Zerva, A.; Topakas, E.; Karampa, P.
Deposited on : 2023-05-12
Resolution : 1.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

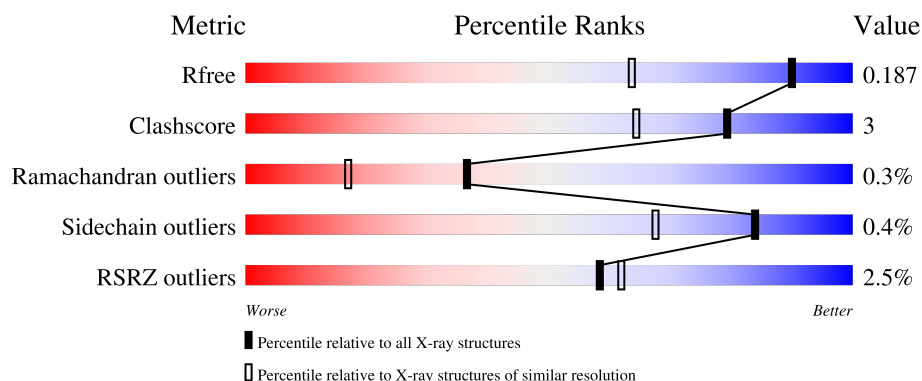
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

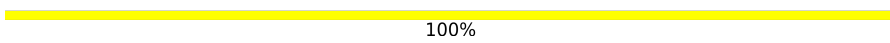
The reported resolution of this entry is 1.42 Å.

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))
R_{free}	180053	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	353	
2	A	2	
3	C	6	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 3085 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 Carbohydrate esterase family 16 protein.

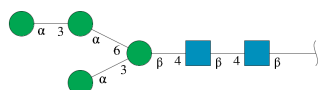
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	323	Total	C	N	O	S	0	5	0
			2570	1635	432	492	11			

There are 26 discrepancies between the modelled and reference sequences:

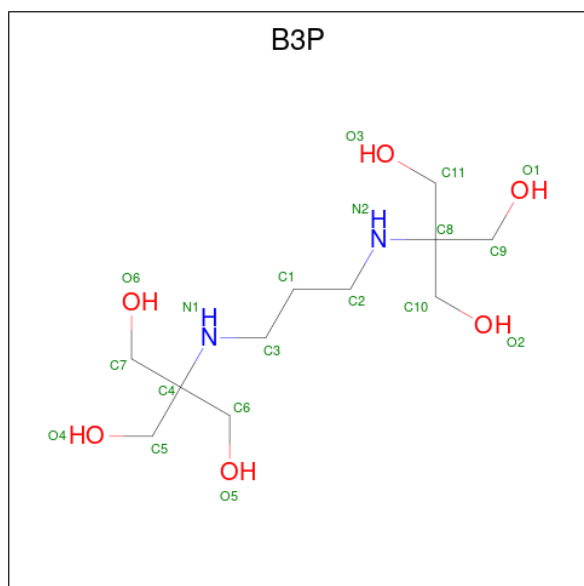
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	expression tag	UNP G2QL32
B	2	ILE	-	expression tag	UNP G2QL32
B	19	ALA	SER	engineered mutation	UNP G2QL32
B	331	ARG	-	expression tag	UNP G2QL32
B	332	LEU	-	expression tag	UNP G2QL32
B	333	GLU	-	expression tag	UNP G2QL32
B	334	GLN	-	expression tag	UNP G2QL32
B	335	LYS	-	expression tag	UNP G2QL32
B	336	LEU	-	expression tag	UNP G2QL32
B	337	ILE	-	expression tag	UNP G2QL32
B	338	SER	-	expression tag	UNP G2QL32
B	339	GLU	-	expression tag	UNP G2QL32
B	340	GLU	-	expression tag	UNP G2QL32
B	341	ASP	-	expression tag	UNP G2QL32
B	342	LEU	-	expression tag	UNP G2QL32
B	343	ASN	-	expression tag	UNP G2QL32
B	344	SER	-	expression tag	UNP G2QL32
B	345	ALA	-	expression tag	UNP G2QL32
B	346	VAL	-	expression tag	UNP G2QL32
B	347	ASP	-	expression tag	UNP G2QL32
B	348	HIS	-	expression tag	UNP G2QL32
B	349	HIS	-	expression tag	UNP G2QL32
B	350	HIS	-	expression tag	UNP G2QL32
B	351	HIS	-	expression tag	UNP G2QL32
B	352	HIS	-	expression tag	UNP G2QL32
B	353	HIS	-	expression tag	UNP G2QL32

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- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-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.

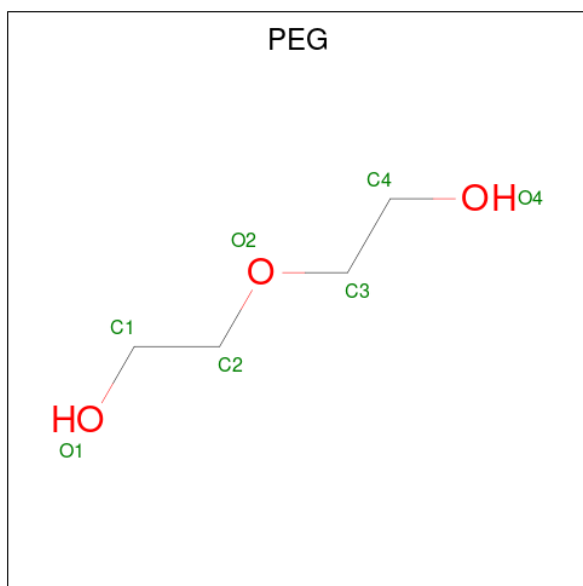


- Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



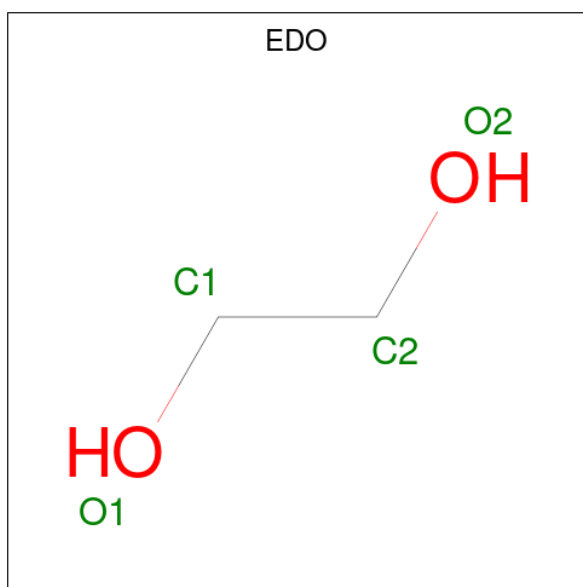
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			5	3	2		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



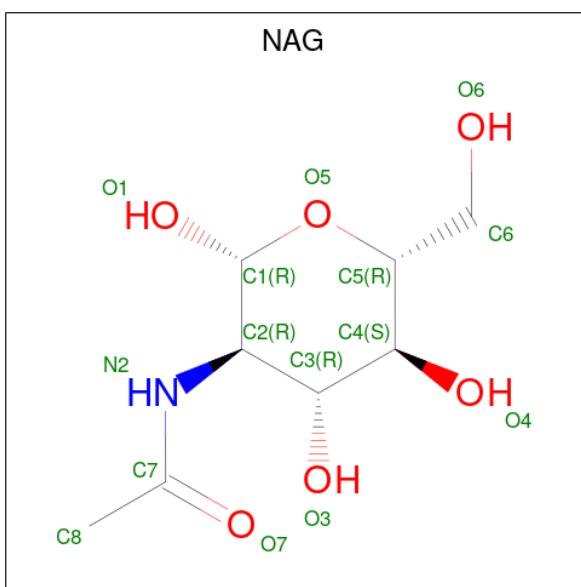
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

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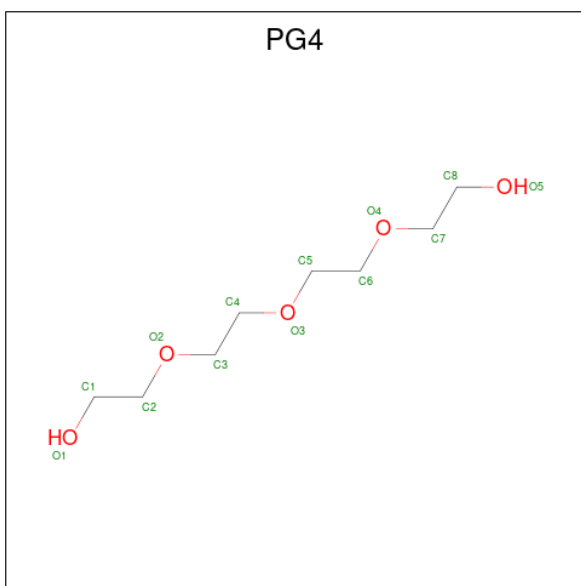
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O		
			13	8	5	0	0

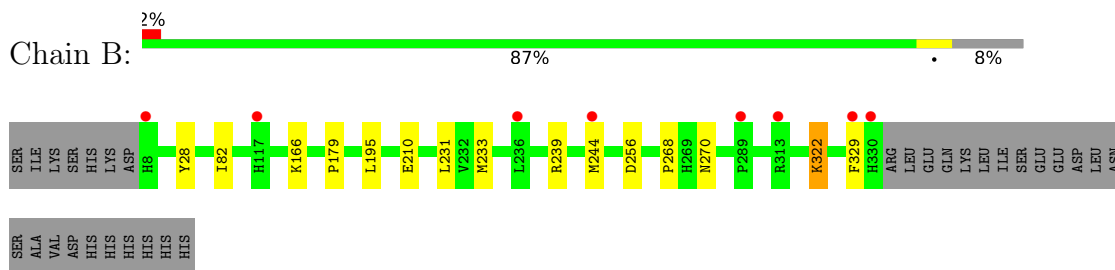
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	275	Total 275	O 275	0	0

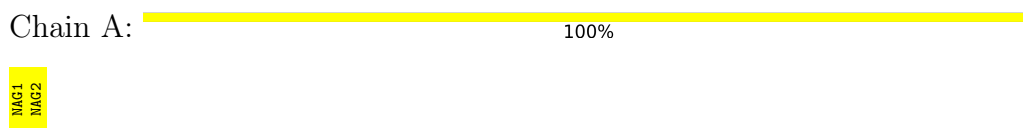
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: Carbohydrate esterase family 16 protein



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



- Molecule 3: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-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



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.54Å 82.54Å 101.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.31 – 1.42 41.31 – 1.42	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.31-1.42) 99.9 (41.31-1.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.167 , 0.183 0.170 , 0.187	Depositor DCC
R_{free} test set	3960 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3085	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: B3P, ACT, MAN, BMA, NAG, EDO, PG4, PEG

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	B	0.99	0/2642	1.10	1/3602 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	179	PRO	N-CA-CB	5.68	106.51	102.65

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	B	2570	0	2439	13	0
2	A	28	0	25	0	0
3	C	72	0	61	0	0
4	B	19	0	26	0	0
5	B	26	0	35	3	0
6	B	12	0	9	1	0
7	B	56	0	84	6	0
8	B	14	0	13	0	0
9	B	13	0	18	0	0
10	B	275	0	0	2	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3085	0	2710	15	2

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 3.

All (15) 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:B:270:ASN:HD22	7:B:408:EDO:H21	1.32	0.94
1:B:210[B]:GLU:OE1	10:B:501:HOH:O	2.02	0.77
1:B:256:ASP:OD1	7:B:404:EDO:H12	2.09	0.53
1:B:239:ARG:HH12	7:B:410:EDO:H21	1.75	0.52
6:B:405:ACT:O	6:B:423:ACT:H2	2.10	0.51
1:B:268:PRO:HB2	7:B:408:EDO:H12	1.94	0.50
5:B:402:PEG:H22	10:B:738:HOH:O	2.12	0.50
1:B:239:ARG:HH12	7:B:410:EDO:C2	2.25	0.49
1:B:166:LYS:NZ	5:B:419:PEG:H31	2.29	0.46
1:B:82[A]:ILE:HD11	5:B:420:PEG:O1	2.17	0.45
1:B:231:LEU:HD13	1:B:329:PHE:CD1	2.52	0.45
1:B:28:TYR:CD1	1:B:28:TYR:C	2.97	0.42
1:B:233:MET:HE3	7:B:410:EDO:H21	2.02	0.42
1:B:244:MET:HE3	1:B:244:MET:HB2	1.89	0.41
1:B:322:LYS:HD2	1:B:322:LYS:O	2.21	0.40

All (2) 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)
10:B:501:HOH:O	10:B:501:HOH:O[4_555]	1.25	0.95
10:B:713:HOH:O	10:B:771:HOH:O[3_665]	2.19	0.01

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	B	326/353 (92%)	315 (97%)	10 (3%)	1 (0%)	36 17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	LEU

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	B	277/301 (92%)	276 (100%)	1 (0%)	84 67

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	322	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	31	ASN
1	B	163	HIS

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 ⓘ

8 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	A	1	2,1	14,14,15	0.67	0	17,19,21	1.02	1 (5%)
2	NAG	A	2	2	14,14,15	0.57	0	17,19,21	1.30	2 (11%)
3	NAG	C	1	3,1	14,14,15	0.63	0	17,19,21	1.02	1 (5%)
3	NAG	C	2	3	14,14,15	0.58	0	17,19,21	0.92	1 (5%)
3	BMA	C	3	3	11,11,12	0.75	0	15,15,17	0.97	1 (6%)
3	MAN	C	4	3	11,11,12	0.63	0	15,15,17	1.02	0
3	MAN	C	5	3	11,11,12	0.40	0	15,15,17	0.96	0
3	MAN	C	6	3	11,11,12	0.93	0	15,15,17	1.15	2 (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
2	NAG	A	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
3	MAN	C	6	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2	NAG	C1-O5-C5	-2.95	108.23	112.19
3	C	1	NAG	C1-O5-C5	2.50	115.53	112.19
2	A	1	NAG	C1-C2-N2	2.40	114.21	110.43
3	C	3	BMA	C1-C2-C3	-2.32	106.26	109.64
2	A	2	NAG	O7-C7-N2	2.27	125.99	121.98
3	C	6	MAN	O5-C1-C2	-2.17	105.61	110.79
3	C	6	MAN	C1-O5-C5	2.07	114.96	112.19
3	C	2	NAG	O4-C4-C3	-2.03	105.58	110.38

There are no chirality outliers.

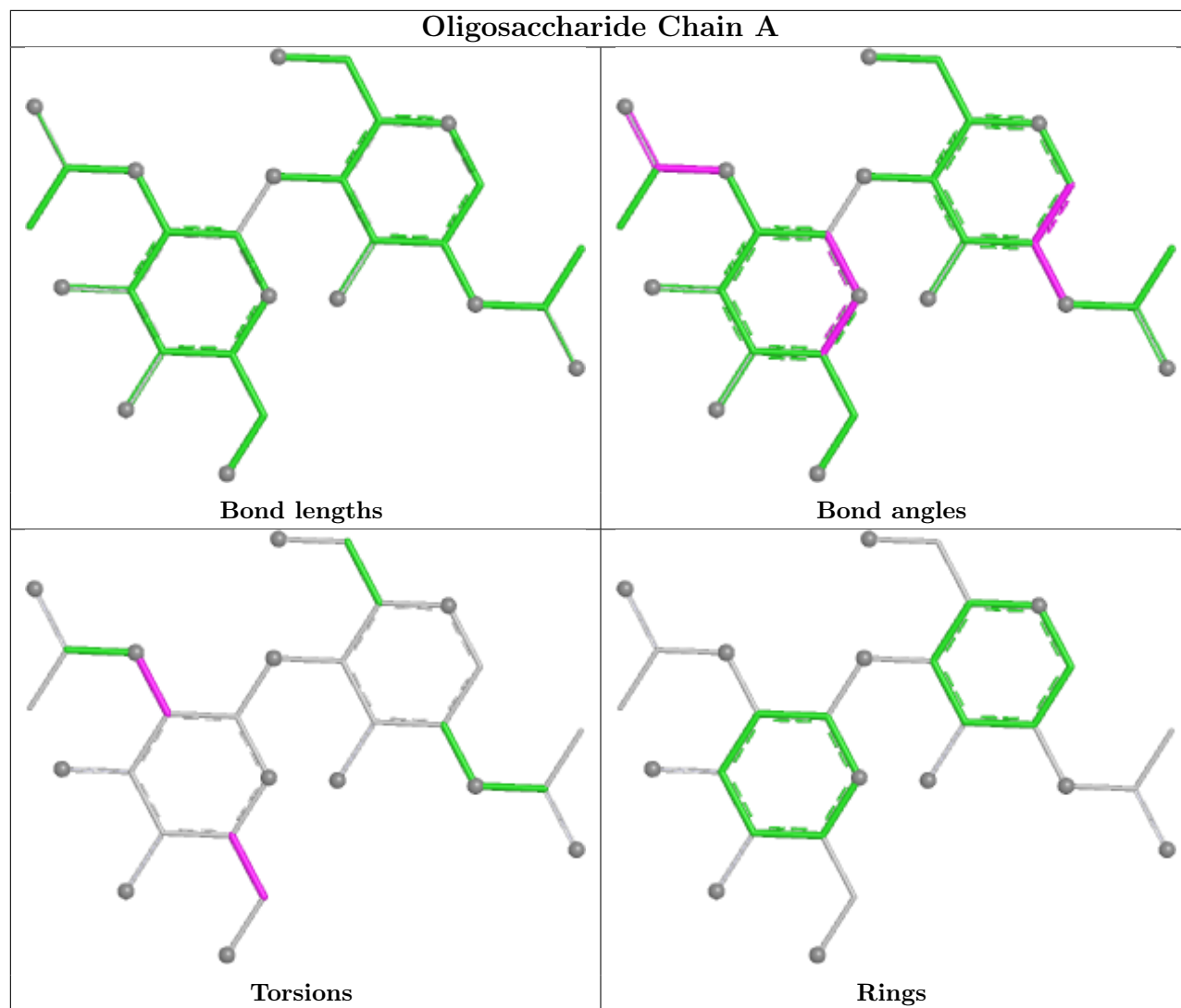
All (10) torsion outliers are listed below:

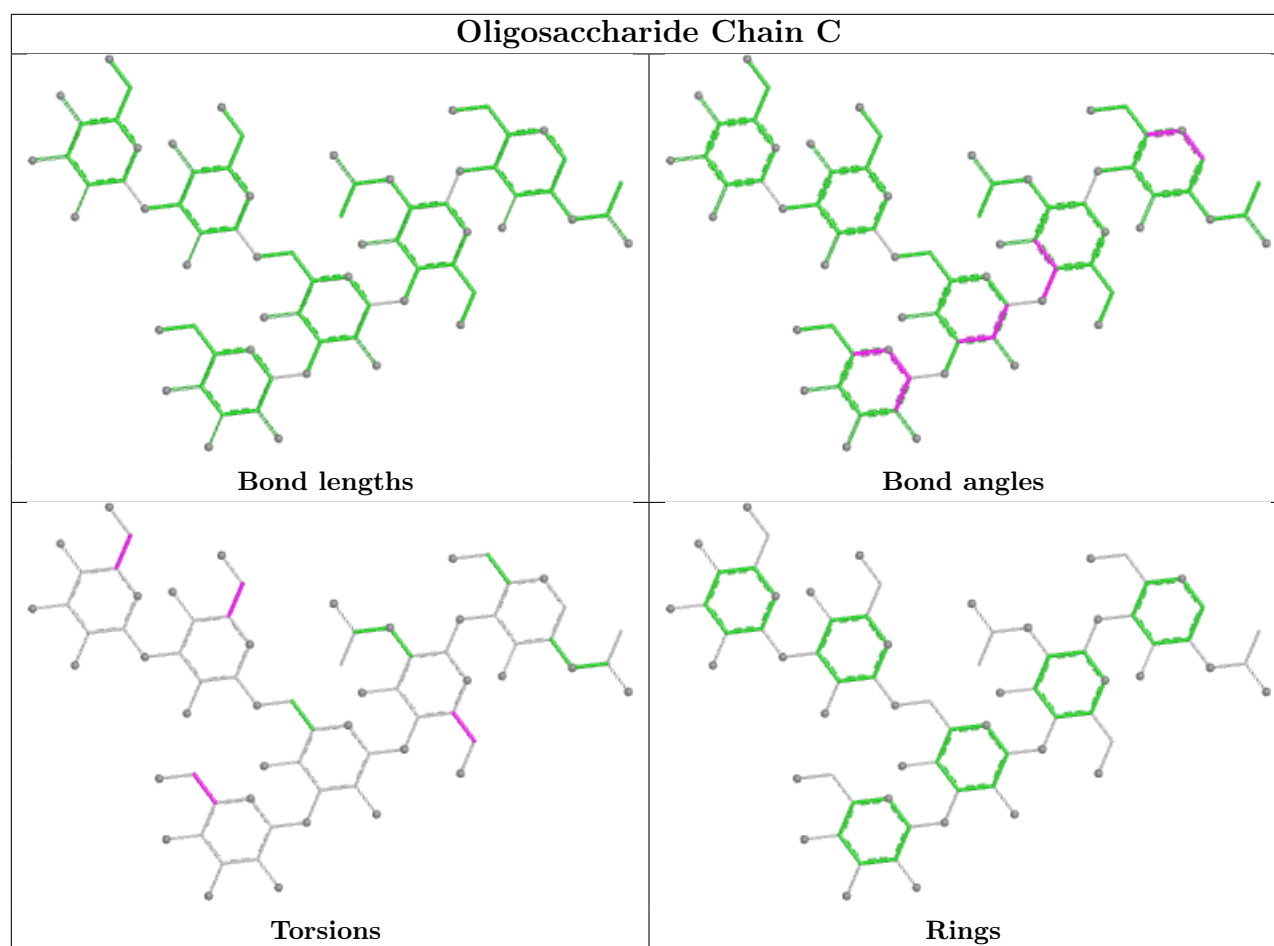
Mol	Chain	Res	Type	Atoms
3	C	5	MAN	O5-C5-C6-O6
3	C	6	MAN	C4-C5-C6-O6
3	C	5	MAN	C4-C5-C6-O6
3	C	6	MAN	O5-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	C	4	MAN	C4-C5-C6-O6
2	A	2	NAG	C1-C2-N2-C7
2	A	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

24 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	$\# Z > 2$
7	EDO	B	408	-	3,3,3	0.09	0	2,2,2	0.43	0
7	EDO	B	407	-	3,3,3	0.07	0	2,2,2	0.18	0
7	EDO	B	411	-	3,3,3	0.10	0	2,2,2	0.17	0
4	B3P	B	401	-	18,18,18	0.21	0	23,23,23	1.01	1 (4%)
7	EDO	B	406	-	3,3,3	0.13	0	2,2,2	0.23	0
5	PEG	B	420	-	6,6,6	0.14	0	5,5,5	0.12	0
5	PEG	B	419	-	4,4,6	0.20	0	3,3,5	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	PG4	B	421	-	12,12,12	0.23	0	11,11,11	0.15	0
7	EDO	B	418	-	3,3,3	0.10	0	2,2,2	0.20	0
7	EDO	B	413	-	3,3,3	0.08	0	2,2,2	0.13	0
7	EDO	B	412	-	3,3,3	0.12	0	2,2,2	0.24	0
7	EDO	B	404	-	3,3,3	0.10	0	2,2,2	0.24	0
6	ACT	B	405	-	3,3,3	1.02	0	3,3,3	0.79	0
7	EDO	B	424	-	3,3,3	0.15	0	2,2,2	0.13	0
5	PEG	B	402	-	6,6,6	0.19	0	5,5,5	0.14	0
7	EDO	B	415	-	3,3,3	0.18	0	2,2,2	0.20	0
5	PEG	B	414	-	6,6,6	0.14	0	5,5,5	0.07	0
7	EDO	B	416	-	3,3,3	0.06	0	2,2,2	0.14	0
7	EDO	B	410	-	3,3,3	0.44	0	2,2,2	0.36	0
7	EDO	B	422	-	3,3,3	0.09	0	2,2,2	0.11	0
6	ACT	B	403	-	3,3,3	1.16	0	3,3,3	0.99	0
6	ACT	B	423	-	3,3,3	0.99	0	3,3,3	0.93	0
8	NAG	B	409	1	14,14,15	0.46	0	17,19,21	1.05	1 (5%)
7	EDO	B	417	-	3,3,3	0.09	0	2,2,2	0.16	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
7	EDO	B	408	-	-	1/1/1/1	-
7	EDO	B	407	-	-	1/1/1/1	-
7	EDO	B	411	-	-	1/1/1/1	-
4	B3P	B	401	-	-	0/28/28/28	-
7	EDO	B	406	-	-	1/1/1/1	-
5	PEG	B	420	-	-	2/4/4/4	-
5	PEG	B	419	-	-	0/2/2/4	-
9	PG4	B	421	-	-	4/10/10/10	-
7	EDO	B	418	-	-	0/1/1/1	-
7	EDO	B	413	-	-	1/1/1/1	-
7	EDO	B	412	-	-	0/1/1/1	-
7	EDO	B	404	-	-	1/1/1/1	-
7	EDO	B	424	-	-	1/1/1/1	-
5	PEG	B	402	-	-	1/4/4/4	-
7	EDO	B	415	-	-	1/1/1/1	-
5	PEG	B	414	-	-	2/4/4/4	-
7	EDO	B	416	-	-	1/1/1/1	-
7	EDO	B	410	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	422	-	-	1/1/1/1	-
8	NAG	B	409	1	-	0/6/23/26	0/1/1/1
7	EDO	B	417	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	409	NAG	O5-C5-C4	-2.54	104.64	110.83
4	B	401	B3P	C5-C4-N1	-2.04	102.92	109.02

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	414	PEG	O2-C3-C4-O4
9	B	421	PG4	O4-C7-C8-O5
5	B	414	PEG	O1-C1-C2-O2
7	B	404	EDO	O1-C1-C2-O2
7	B	407	EDO	O1-C1-C2-O2
5	B	420	PEG	O1-C1-C2-O2
9	B	421	PG4	O2-C3-C4-O3
5	B	402	PEG	O1-C1-C2-O2
7	B	408	EDO	O1-C1-C2-O2
7	B	417	EDO	O1-C1-C2-O2
7	B	424	EDO	O1-C1-C2-O2
7	B	413	EDO	O1-C1-C2-O2
9	B	421	PG4	C1-C2-O2-C3
9	B	421	PG4	O3-C5-C6-O4
7	B	416	EDO	O1-C1-C2-O2
7	B	411	EDO	O1-C1-C2-O2
7	B	415	EDO	O1-C1-C2-O2
7	B	422	EDO	O1-C1-C2-O2
5	B	420	PEG	O2-C3-C4-O4
7	B	406	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 10 short contacts:

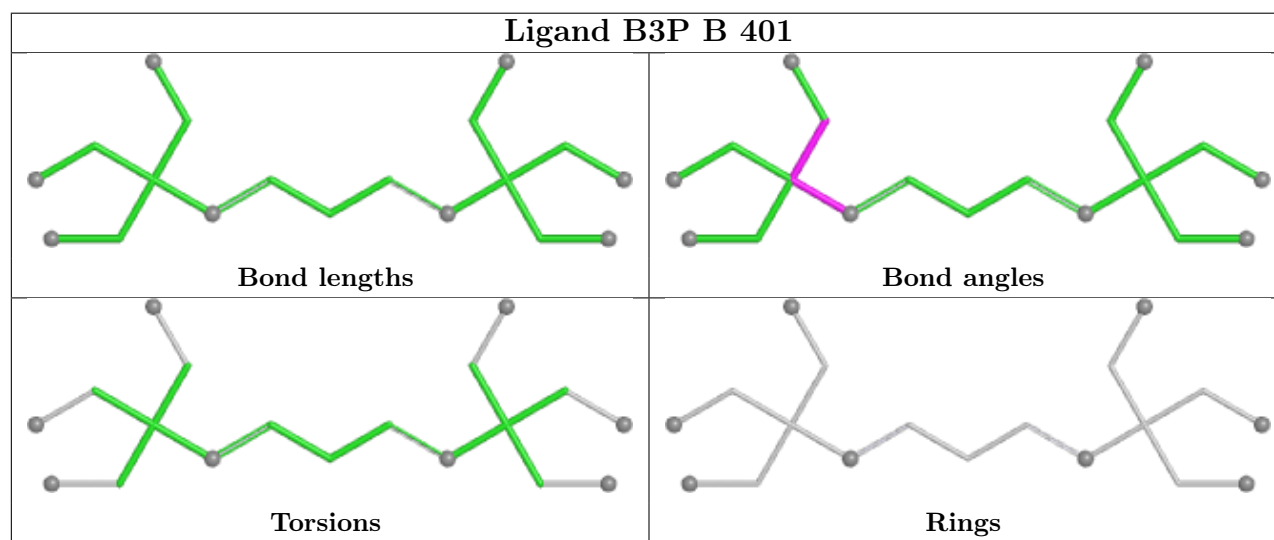
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	408	EDO	2	0

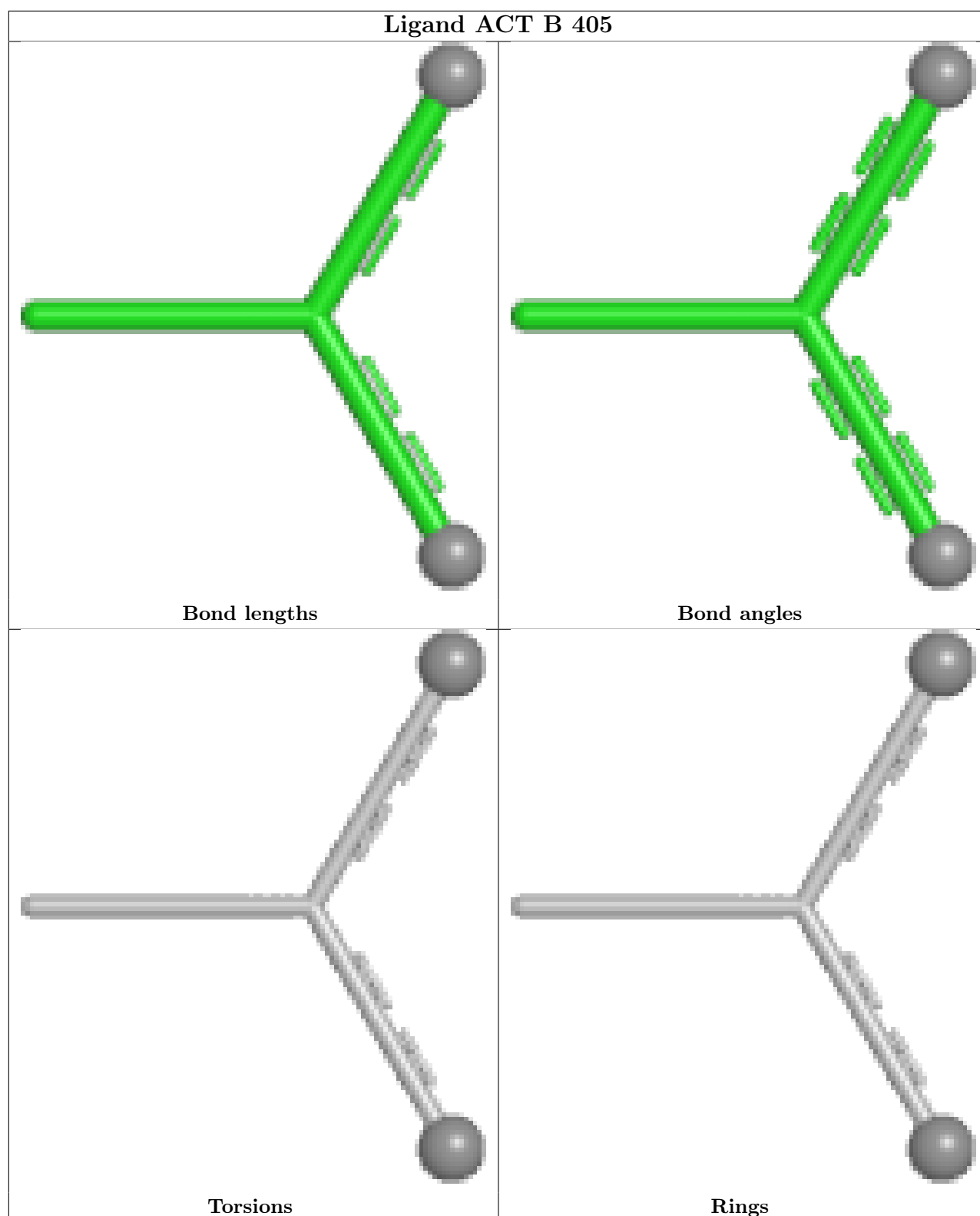
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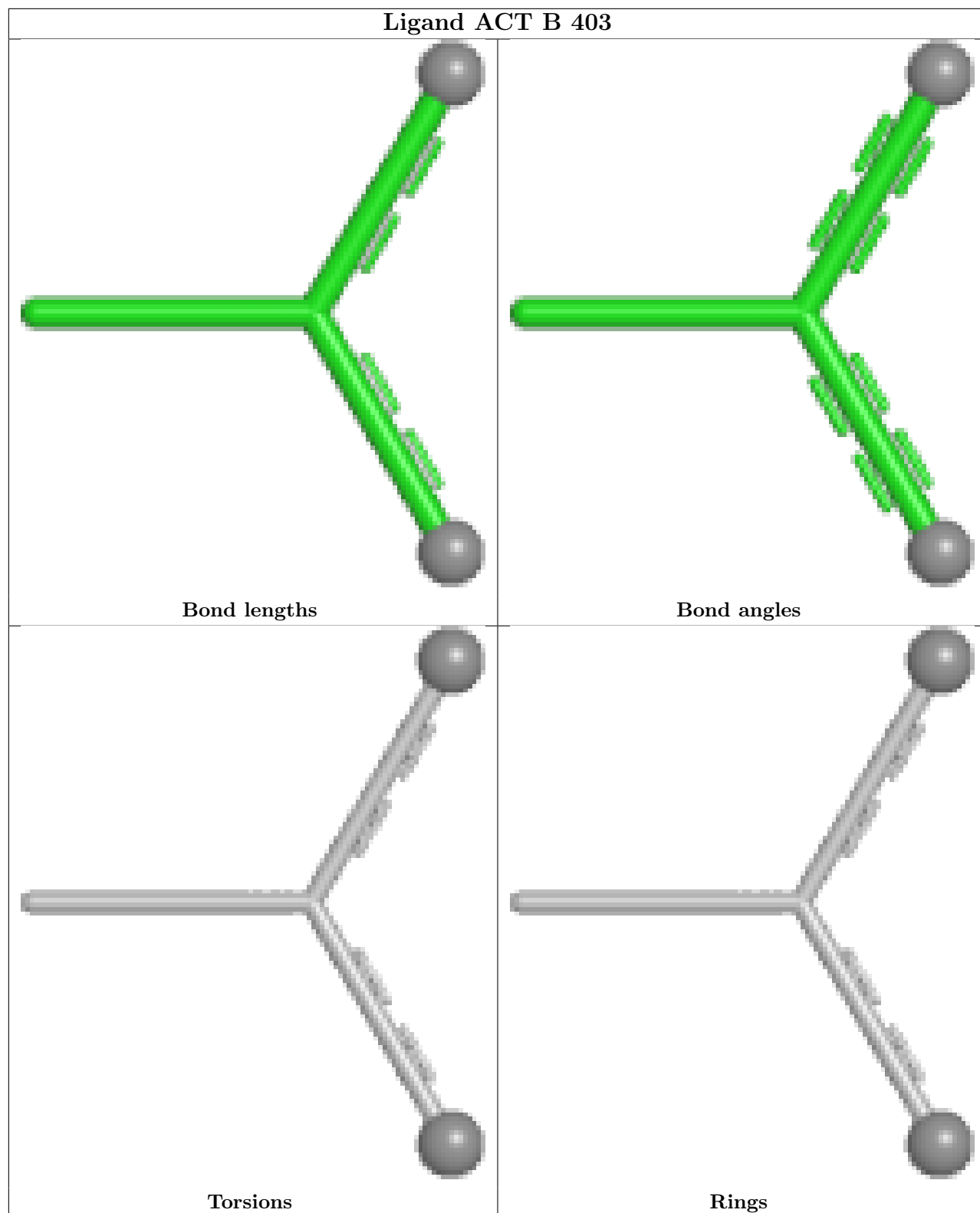
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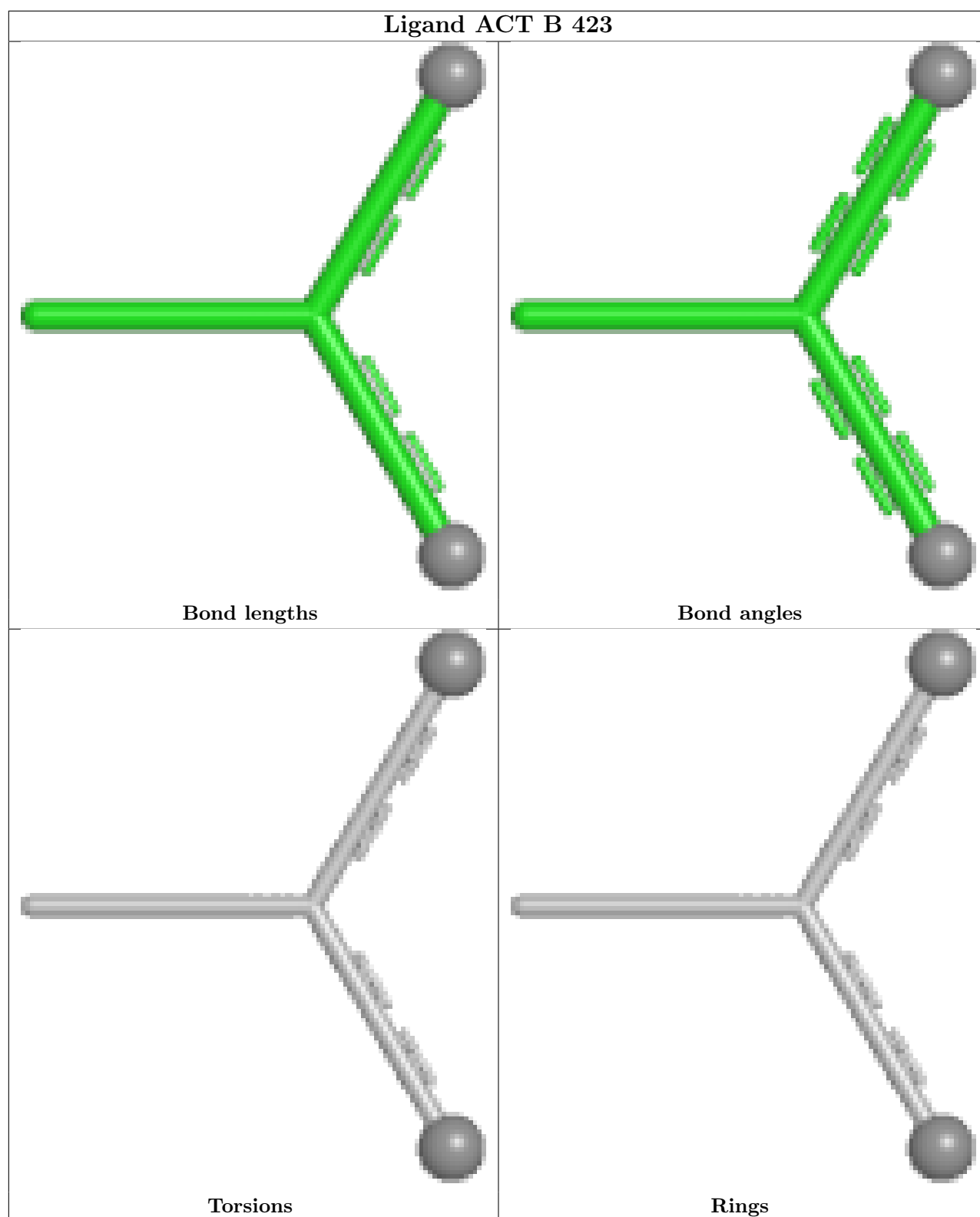
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	420	PEG	1	0
5	B	419	PEG	1	0
7	B	404	EDO	1	0
6	B	405	ACT	1	0
5	B	402	PEG	1	0
7	B	410	EDO	3	0
6	B	423	ACT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	323/353 (91%)	0.11	8 (2%) 58 62	8, 21, 37, 47	5 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	236	LEU	3.6
1	B	289	PRO	3.0
1	B	313	ARG	2.9
1	B	330	HIS	2.6
1	B	244	MET	2.3
1	B	8	HIS	2.2
1	B	329	PHE	2.0
1	B	117	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

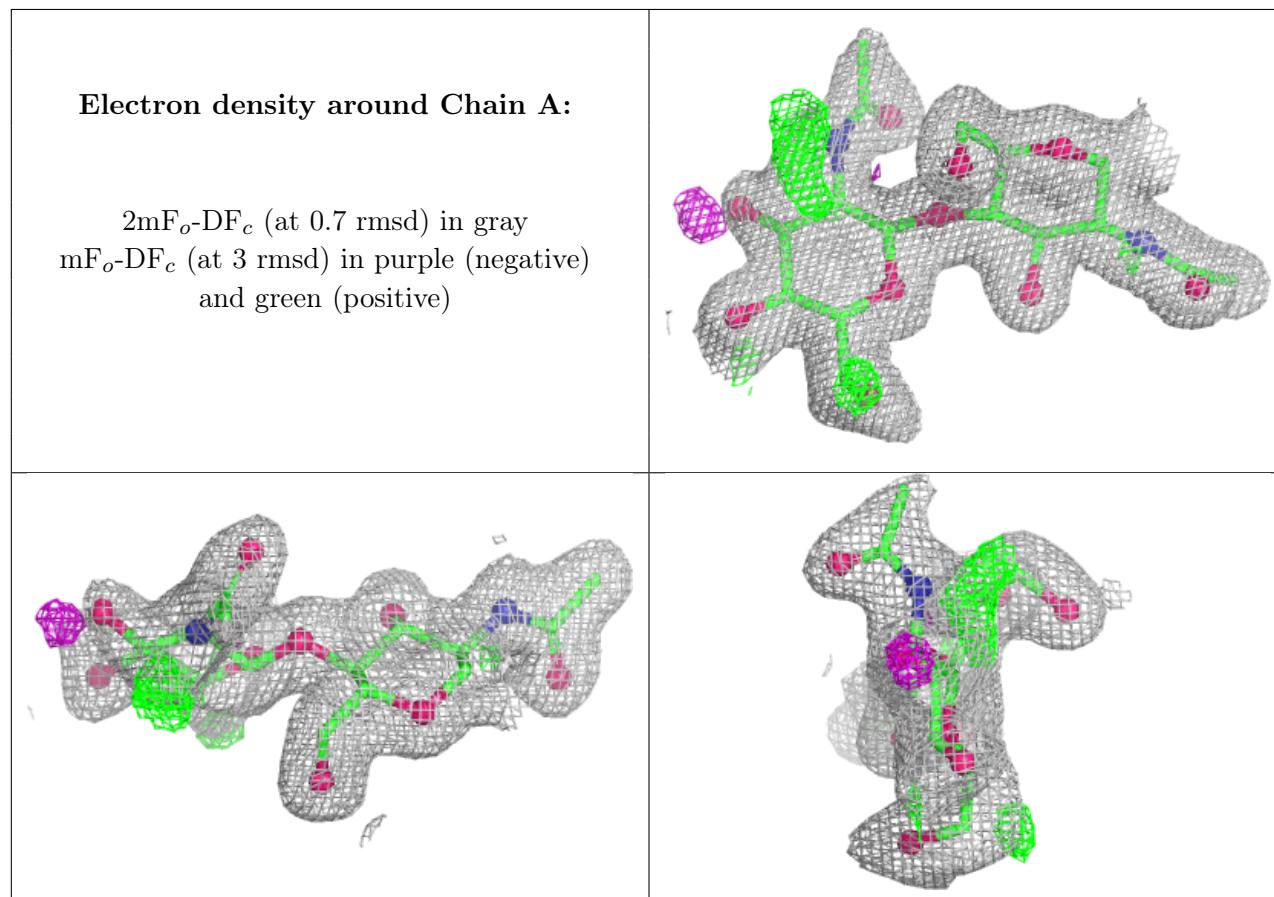
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	1	14/15	-	-	23,26,29,32	0
2	NAG	A	2	14/15	-	-	35,39,44,46	0
3	MAN	C	6	11/12	0.69	0.17	38,40,43,46	0
3	MAN	C	4	11/12	0.82	0.13	33,36,45,49	0

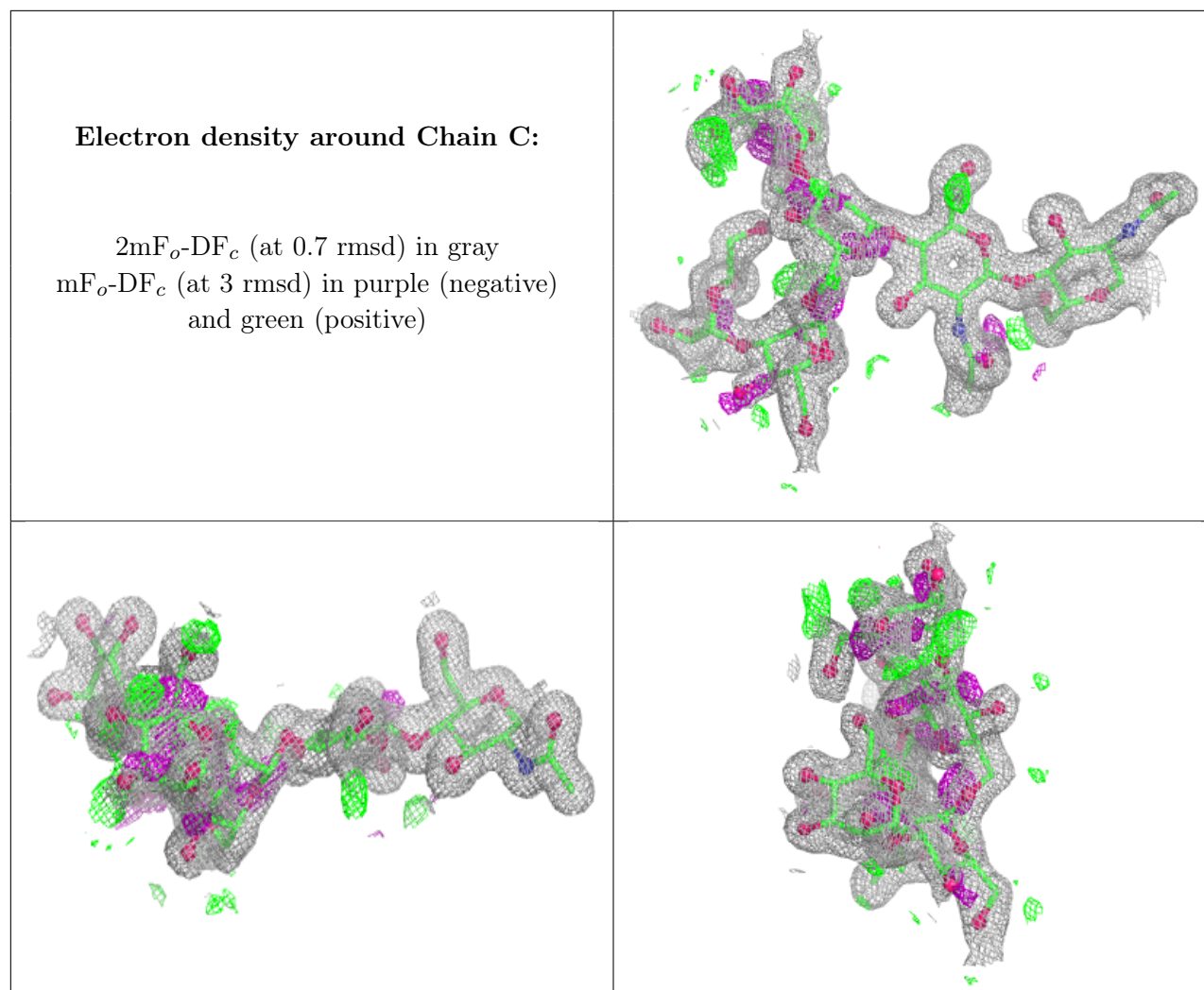
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	C	3	11/12	0.85	0.13	29,33,36,41	0
3	MAN	C	5	11/12	0.90	0.10	24,34,39,45	0
3	NAG	C	2	14/15	0.91	0.10	24,26,28,32	0
3	NAG	C	1	14/15	0.98	0.08	17,18,19,20	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	ACT	B	405	4/4	0.45	0.24	58,58,61,64	0
8	NAG	B	409	14/15	0.55	0.17	57,71,74,77	0
7	EDO	B	406	4/4	0.67	0.17	49,56,59,63	0
6	ACT	B	423	4/4	0.70	0.17	49,52,57,59	0
7	EDO	B	411	4/4	0.71	0.19	55,56,56,59	0
7	EDO	B	422	4/4	0.76	0.18	69,69,71,72	0
7	EDO	B	416	4/4	0.77	0.20	64,64,67,70	0
7	EDO	B	418	4/4	0.77	0.20	59,63,64,65	0
5	PEG	B	414	7/7	0.78	0.21	54,59,62,63	0

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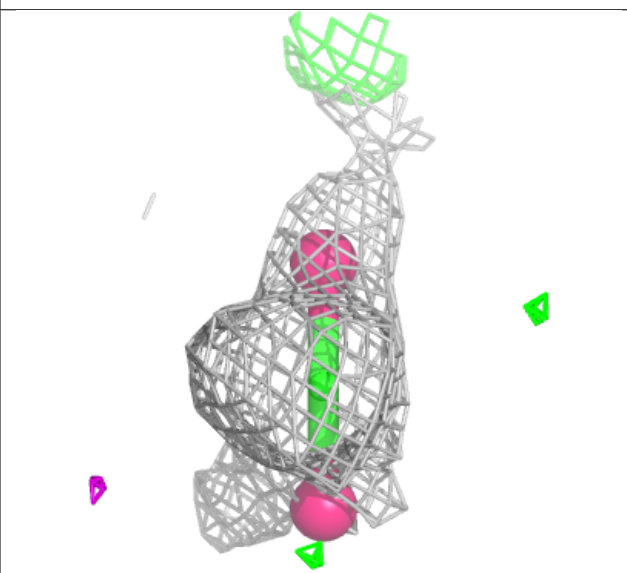
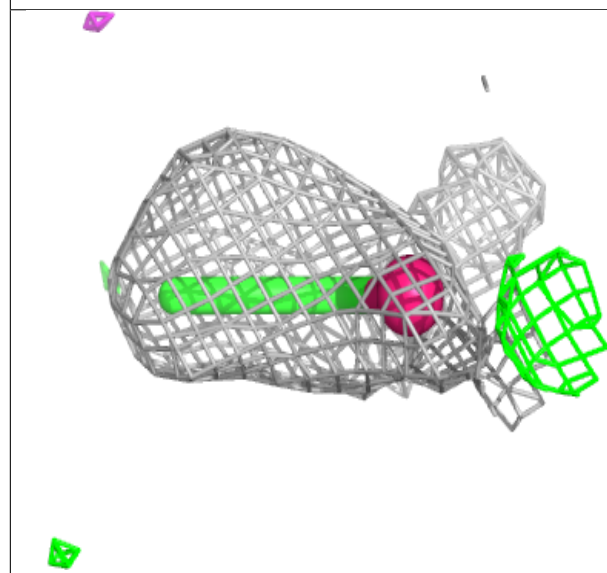
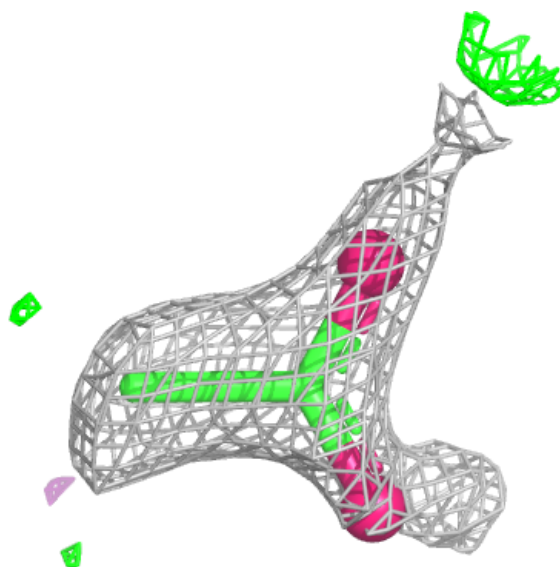
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	B	410	4/4	0.81	0.15	34,43,43,47	0
9	PG4	B	421	13/13	0.81	0.17	51,53,55,56	0
7	EDO	B	413	4/4	0.83	0.19	60,62,65,68	0
7	EDO	B	407	4/4	0.83	0.16	41,50,51,53	0
7	EDO	B	408	4/4	0.84	0.13	43,44,48,51	0
5	PEG	B	420	7/7	0.85	0.17	47,56,58,62	0
5	PEG	B	419	5/7	0.85	0.14	34,38,40,44	0
7	EDO	B	417	4/4	0.87	0.15	58,59,60,60	0
7	EDO	B	415	4/4	0.88	0.12	35,36,39,40	0
4	B3P	B	401	19/19	0.89	0.11	19,28,40,44	0
7	EDO	B	424	4/4	0.89	0.13	45,45,49,51	0
7	EDO	B	404	4/4	0.89	0.11	34,36,43,47	0
5	PEG	B	402	7/7	0.89	0.12	42,45,50,53	0
7	EDO	B	412	4/4	0.90	0.11	37,46,46,52	0
6	ACT	B	403	4/4	0.98	0.06	15,19,19,21	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

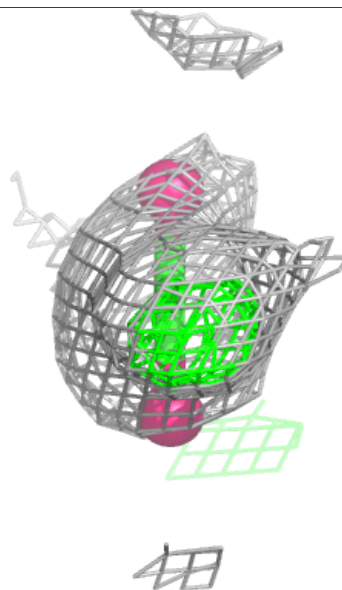
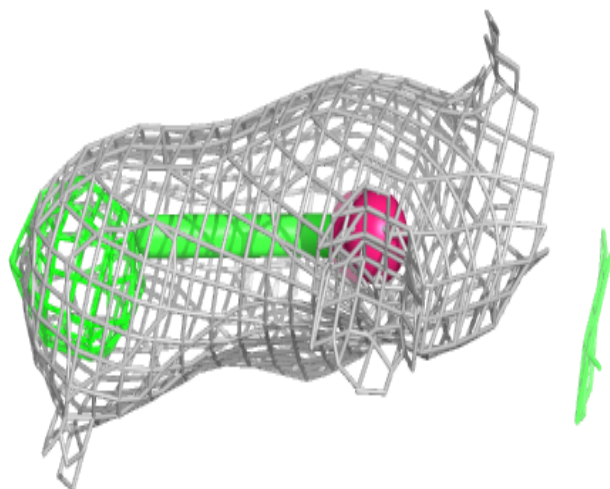
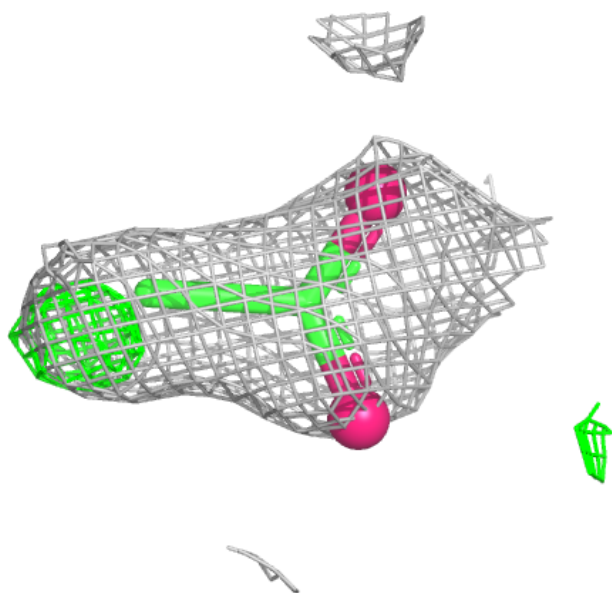
Electron density around ACT B 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



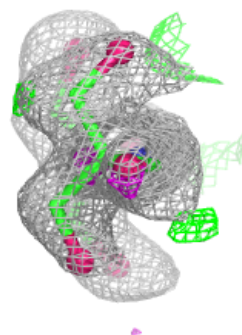
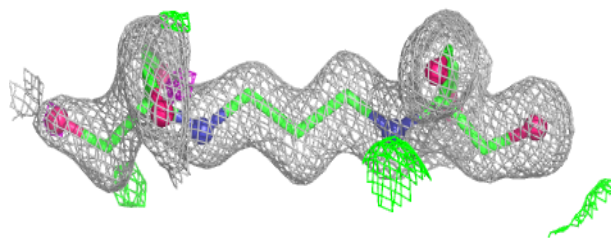
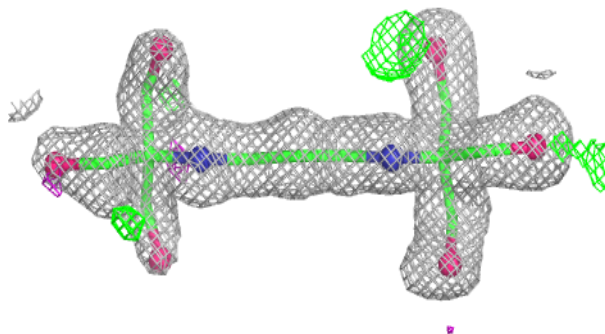
Electron density around ACT B 423:

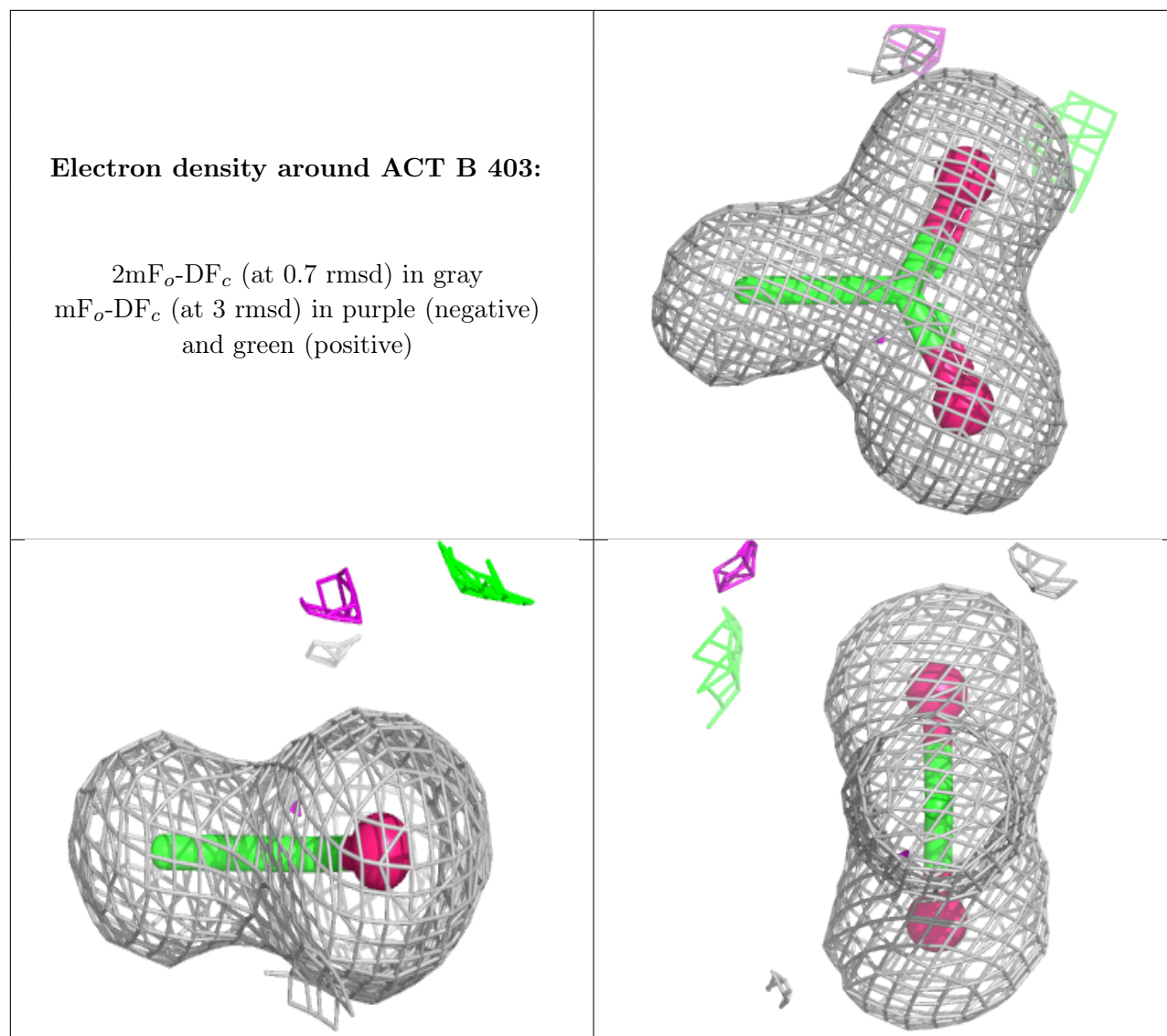
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around B3P B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.