

wwPDB X-ray Structure Validation Summary Report (i)

Mar 12, 2024 – 09:13 am GMT

PDB ID : 8P1G

Title: Crystal structure of inactive TtCE16 in complex with acetate

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Ρ.

Deposited on : 2023-05-12

Resolution : 1.42 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.orgA 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS: 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

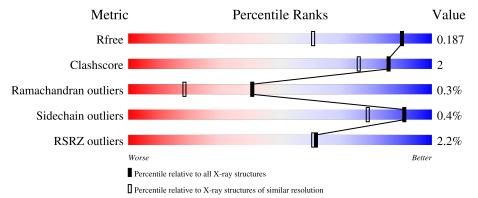
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (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 <=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	В	353	2%	88%	• 8%
2	A	2		100%	
3	С	6	33%	67%	



2 Entry composition (i)

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.

\mathbf{Mol}	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	В	323	Total 2570	C 1635	N 432	O 492	S 11	0	5	0

There are 26 discrepancies between the modelled and reference sequences:

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

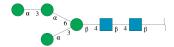


• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



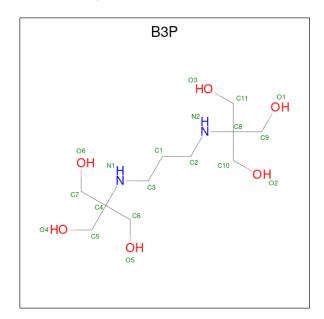
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	A	2	Total 28	C 16	N 2	O 10	0	0	0

• 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.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
3	С	6	Total 72	C 40	N 2	O 30	0	0	0

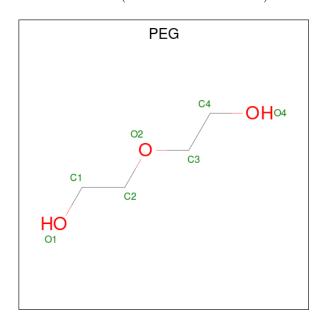
• Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).





\mathbf{Mol}	Chain	Residues	A	Aton	\mathbf{as}		ZeroOcc	AltConf
1	В	1	Total	С	N	О	0	0
4	Б	1	19	11	2	6	0	0

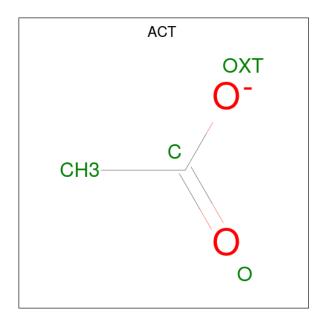
• Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

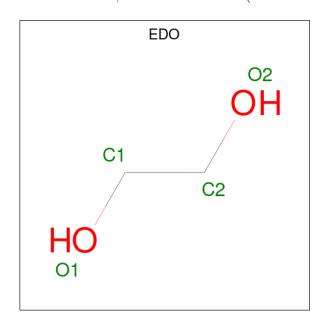
• Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).





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

 \bullet Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



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

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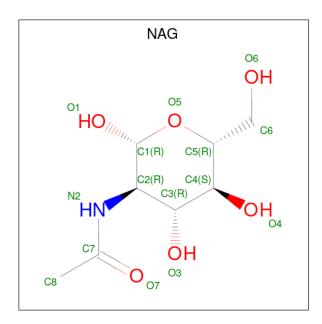


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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	1	Total C O 4 2 2	0	0
7	В	1	Total C O 4 2 2	0	0
7	В	1	Total C O 4 2 2	0	0
7	В	1	Total C O 4 2 2	0	0
7	В	1	Total C O 4 2 2	0	0
7	В	1	Total C O 4 2 2	0	0
7	В	1	Total C O 4 2 2	0	0
7	В	1	Total C O 4 2 2	0	0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

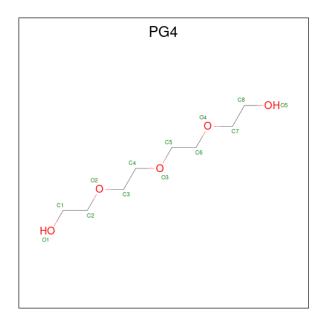
 \bullet Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6).$





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

 \bullet Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $\mathrm{C_8H_{18}O_5}).$



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

• Molecule 10 is water.



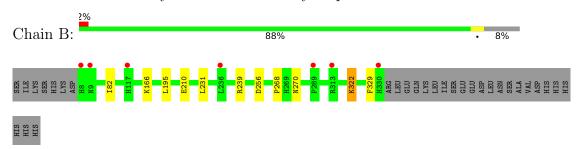
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	В	275	Total O 275 275	0	0



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

Chain A: 100%

 \bullet 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

Chain C: 33% 67%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	82.54Å 82.54Å 101.07Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.31 - 1.42	Depositor
Resolution (A)	41.27 - 1.42	EDS
% Data completeness	100.0 (41.31-1.42)	Depositor
(in resolution range)	99.9 (41.27-1.42)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.31 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.167 , 0.183	Depositor
$\Pi,\ \Pi_{free}$	0.170 , 0.187	DCC
R_{free} test set	3957 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, 45.2	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.34$	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.

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



¹Intensities estimated from amplitudes.

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

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).

Mal	Chain	Bond	lengths	Bond	angles
MIOI	Chain	RMSZ	# Z > 5	RMSZ $\mid \# Z > 5$	
1	В	0.70	0/2642	0.79	0/3602

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	В	2570	0	2439	10	0
2	A	28	0	25	0	0
3	С	72	0	61	0	0
4	В	19	0	26	0	0
5	В	26	0	35	3	0
6	В	12	0	9	1	0
7	В	56	0	84	5	0
8	В	14	0	13	0	0
9	В	13	0	18	0	0
10	В	275	0	0	2	2
All	All	3085	0	2710	12	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 2.



The worst 5 of 12 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ (\rm \AA) \end{array}$	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

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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	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 (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	В	$326/353 \ (92\%)$	315 (97%)	10 (3%)	1 (0%)	41 18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	195	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.



The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	В	277/301 (92%)	276 (100%)	1 (0%)	91 79

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

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	Bo	ond leng	ths	В	ond ang	cles
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1	2,1	14,14,15	0.68	0	17,19,21	1.03	1 (5%)
2	NAG	A	2	2	14,14,15	0.55	0	17,19,21	1.34	3 (17%)



Mol	Tuno	Chain	Res	Link	Вс	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	С	1	3,1	14,14,15	0.64	0	17,19,21	1.03	1 (5%)
3	NAG	С	2	3	14,14,15	0.57	0	17,19,21	0.92	1 (5%)
3	BMA	С	3	3	11,11,12	0.76	0	15,15,17	1.09	1 (6%)
3	MAN	С	4	3	11,11,12	0.64	0	15,15,17	1.12	0
3	MAN	С	5	3	11,11,12	0.41	0	15,15,17	1.03	0
3	MAN	С	6	3	11,11,12	0.93	0	15,15,17	1.38	3 (20%)

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	-	1/6/23/26	0/1/1/1
3	NAG	С	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	С	2	3	-	1/6/23/26	0/1/1/1
3	BMA	С	3	3	-	0/2/19/22	0/1/1/1
3	MAN	С	4	3	-	2/2/19/22	0/1/1/1
3	MAN	С	5	3	-	2/2/19/22	0/1/1/1
3	MAN	С	6	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$\operatorname{Ideal}(^{o})$
3	С	6	MAN	O5-C1-C2	-3.34	105.61	110.77
2	A	2	NAG	C1-O5-C5	-2.92	108.23	112.19
3	С	3	BMA	C1-C2-C3	-2.77	106.26	109.67
3	С	1	NAG	C1-O5-C5	2.47	115.53	112.19
2	A	2	NAG	O5-C5-C6	2.37	110.92	107.20

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	5	MAN	O5-C5-C6-O6
3	С	6	MAN	C4-C5-C6-O6
3	С	5	MAN	C4-C5-C6-O6
3	С	6	MAN	O5-C5-C6-O6

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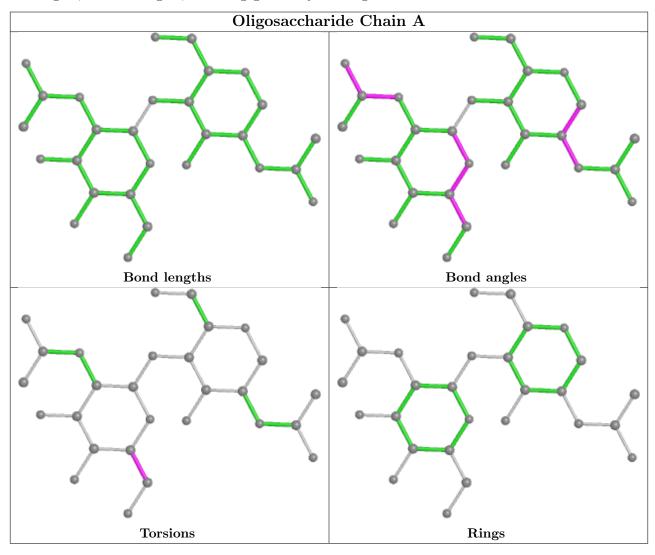
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\mathbf{Mol}	Chain	Res	Type	Atoms
3	С	4	MAN	O5-C5-C6-O6

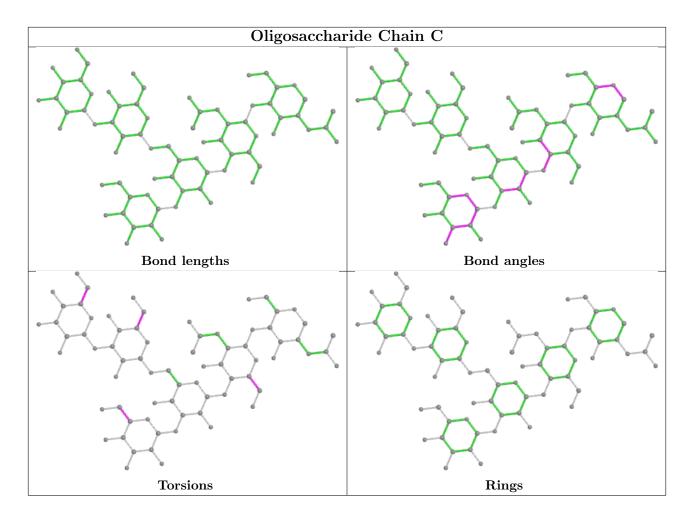
There are no ring outliers.

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	Trino	Chain	Dag	Bond lengths				Bond angles		
MIOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	В	412	-	3,3,3	0.11	0	2,2,2	0.30	0
9	PG4	В	421	-	12,12,12	0.23	0	11,11,11	0.16	0
5	PEG	В	402	-	6,6,6	0.19	0	5,5,5	0.14	0
8	NAG	В	409	1	14,14,15	0.44	0	17,19,21	1.07	1 (5%)
6	ACT	В	423	-	3,3,3	0.94	0	3,3,3	0.93	0
7	EDO	В	416	-	3,3,3	0.06	0	2,2,2	0.21	0
7	EDO	В	422	-	3,3,3	0.08	0	2,2,2	0.14	0



N / - 1	Т	Clasica	Das	Link	Во	ond leng	ths	В	ond ang	eles
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	В	406	-	3,3,3	0.13	0	2,2,2	0.31	0
5	PEG	В	414	-	6,6,6	0.14	0	5,5,5	0.07	0
6	ACT	В	403	-	3,3,3	1.10	0	3,3,3	0.99	0
7	EDO	В	413	-	3,3,3	0.07	0	2,2,2	0.20	0
7	EDO	В	415	-	3,3,3	0.19	0	2,2,2	0.27	0
5	PEG	В	419	-	4,4,6	0.21	0	3,3,5	0.14	0
6	ACT	В	405	-	3,3,3	0.96	0	3,3,3	0.78	0
7	EDO	В	404	-	3,3,3	0.10	0	2,2,2	0.32	0
7	EDO	В	418	-	3,3,3	0.10	0	2,2,2	0.28	0
7	EDO	В	411	-	3,3,3	0.11	0	2,2,2	0.23	0
5	PEG	В	420	-	6,6,6	0.14	0	5,5,5	0.12	0
4	ВЗР	В	401	-	18,18,18	0.20	0	21,23,23	1.07	1 (4%)
7	EDO	В	407	-	3,3,3	0.07	0	2,2,2	0.25	0
7	EDO	В	424	-	3,3,3	0.15	0	2,2,2	0.20	0
7	EDO	В	410	-	3,3,3	0.44	0	2,2,2	0.38	0
7	EDO	В	408	-	3,3,3	0.10	0	2,2,2	0.50	0
7	EDO	В	417	-	3,3,3	0.09	0	2,2,2	0.21	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	В	412	-	-	0/1/1/1	-
9	PG4	В	421	-	-	4/10/10/10	-
5	PEG	В	402	-	-	1/4/4/4	-
8	NAG	В	409	1	-	0/6/23/26	0/1/1/1
7	EDO	В	416	_	-	1/1/1/1	-
7	EDO	В	422	_	-	1/1/1/1	-
7	EDO	В	406	_	-	1/1/1/1	-
5	PEG	В	414	_	-	2/4/4/4	-
7	EDO	В	413	-	-	1/1/1/1	-
7	EDO	В	415	-	-	1/1/1/1	-
5	PEG	В	419	-	-	0/2/2/4	-
7	EDO	В	404	-	-	1/1/1/1	-
7	EDO	В	418	-	-	0/1/1/1	-
7	EDO	В	411	-	-	1/1/1/1	-
5	PEG	В	420	-	-	2/4/4/4	-
4	ВЗР	В	401	-	-	0/28/28/28	-
7	EDO	В	407	-	-	1/1/1/1	-
7	EDO	В	424	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	В	410	-	-	0/1/1/1	-
7	EDO	В	408	-	-	1/1/1/1	-
7	EDO	В	417	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathrm{Ideal}(^{o})$
8	В	409	NAG	O5-C5-C4	-2.54	104.64	110.83
4	В	401	ВЗР	C5-C4-N1	-2.03	102.92	109.03

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	414	PEG	O2-C3-C4-O4
9	В	421	PG4	O4-C7-C8-O5
5	В	414	PEG	O1-C1-C2-O2
7	В	404	EDO	O1-C1-C2-O2
7	В	407	EDO	O1-C1-C2-O2

There are no ring outliers.

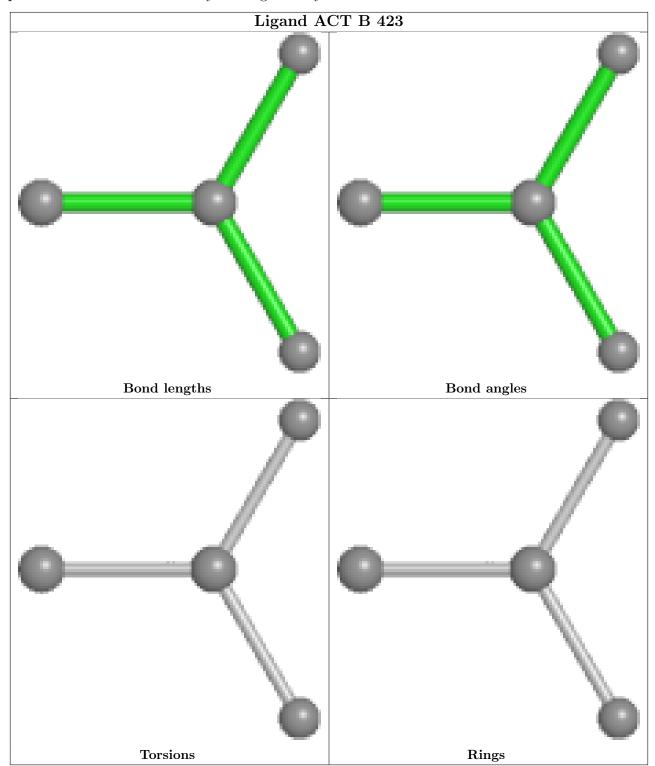
8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	В	402	PEG	1	0
6	В	423	ACT	1	0
5	В	419	PEG	1	0
6	В	405	ACT	1	0
7	В	404	EDO	1	0
5	В	420	PEG	1	0
7	В	410	EDO	2	0
7	В	408	EDO	2	0

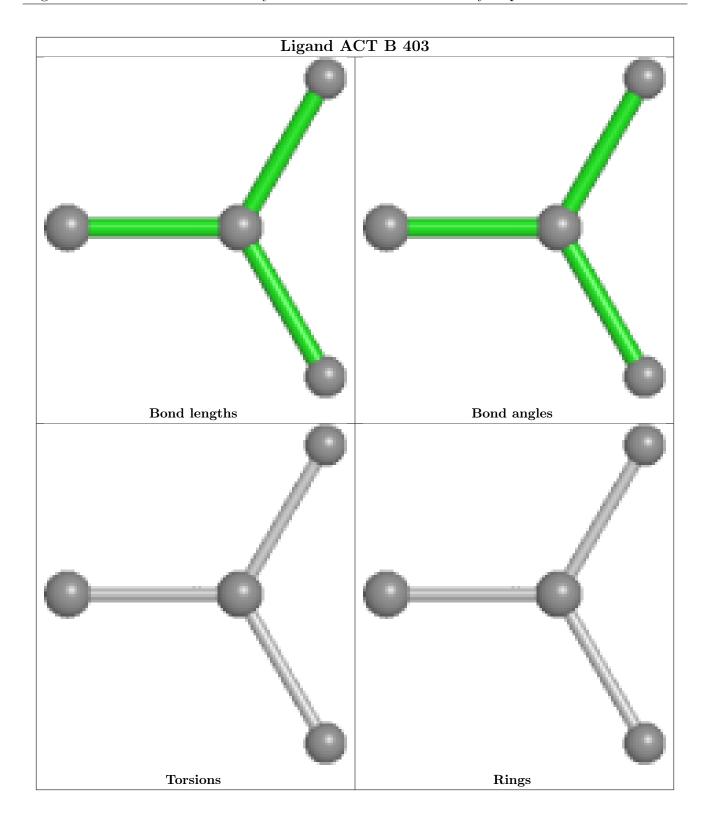
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



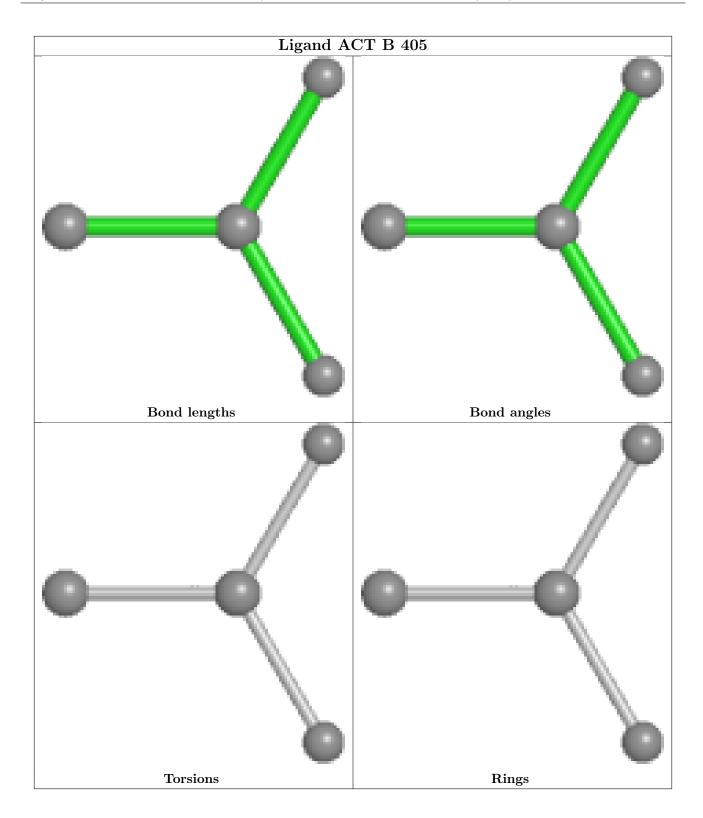
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



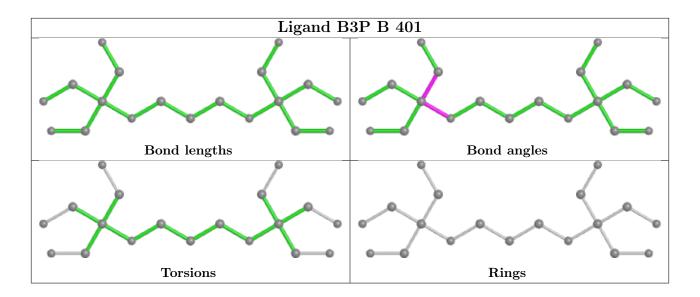












5.7 Other polymers (i)

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 (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, 95^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$		$OWAB(Å^2)$	Q<0.9	
1	В	323/353 (91%)	-0.03	7 (2%)	62	61	15, 21, 37, 47	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	289	PRO	3.0
1	В	9	ASN	3.0
1	В	8	HIS	3.0
1	В	313	ARG	2.9
1	В	330	HIS	2.5

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, 95^{th} 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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
3	MAN	С	6	11/12	0.62	0.22	38,40,43,46	0
3	MAN	С	4	11/12	0.81	0.17	33,36,45,49	0
3	BMA	С	3	11/12	0.84	0.19	29,33,36,41	0
2	NAG	A	2	14/15	0.85	0.19	35,39,44,46	0
3	MAN	С	5	11/12	0.89	0.15	24,34,39,45	0
3	NAG	С	2	14/15	0.93	0.09	24,26,28,32	0
2	NAG	A	1	14/15	0.95	0.08	23,26,29,32	0

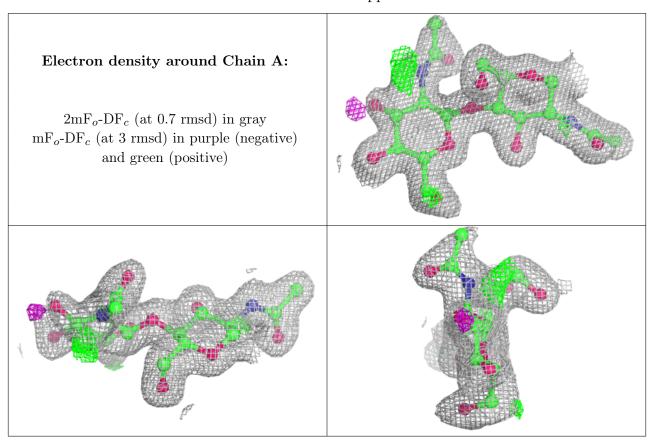
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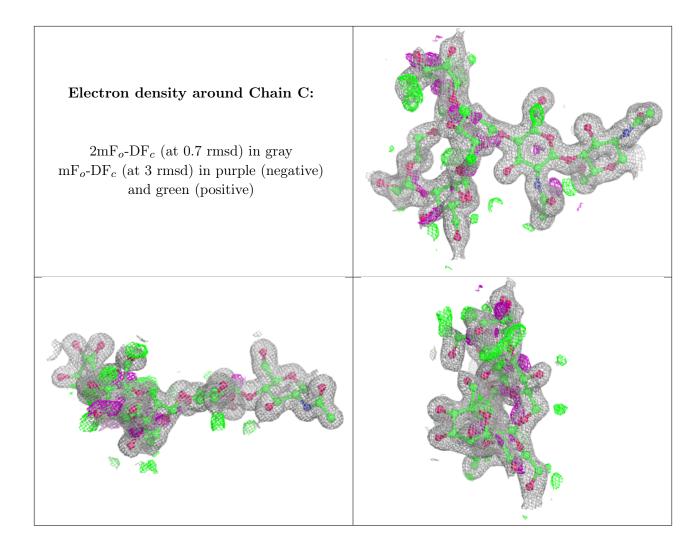
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Mo	l Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	NAG	С	1	14/15	0.98	0.10	17,18,19,20	0

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, 95^{th} 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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
7	EDO	В	416	4/4	0.57	0.18	64,64,67,70	0
6	ACT	В	405	4/4	0.59	0.27	58,58,61,64	0
6	ACT	В	423	4/4	0.61	0.25	49,52,57,59	0
5	PEG	В	414	7/7	0.65	0.27	54,59,62,63	0
7	EDO	В	418	4/4	0.72	0.22	59,63,64,65	0
8	NAG	В	409	14/15	0.74	0.32	57,71,74,77	0
5	PEG	В	420	7/7	0.75	0.15	47,56,58,62	0
7	EDO	В	422	4/4	0.76	0.13	69,69,71,72	0
9	PG4	В	421	13/13	0.76	0.15	51,53,55,56	0
7	EDO	В	417	4/4	0.78	0.15	58,59,60,60	0

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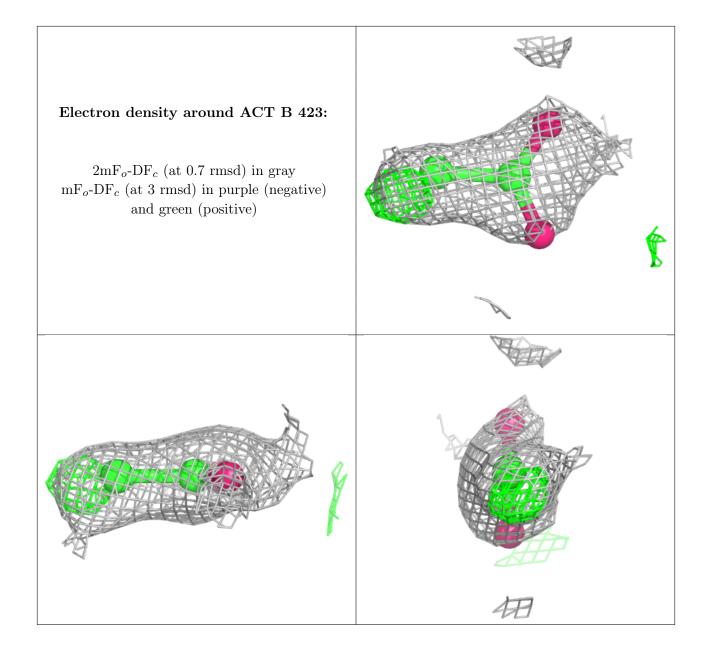
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
7	EDO	В	411	4/4	0.79	0.21	55,56,56,59	0
7	EDO	В	408	4/4	0.80	0.24	43,44,48,51	0
7	EDO	В	413	4/4	0.82	0.14	60,62,65,68	0
7	EDO	В	404	4/4	0.84	0.20	34,36,43,47	0
7	EDO	В	410	4/4	0.85	0.25	34,43,43,47	0
7	EDO	В	407	4/4	0.85	0.18	41,50,51,53	0
5	PEG	В	402	7/7	0.85	0.11	42,45,50,53	0
7	EDO	В	406	4/4	0.86	0.28	49,56,59,63	0
7	EDO	В	412	4/4	0.89	0.24	37,46,46,52	0
5	PEG	В	419	5/7	0.90	0.11	34,38,40,44	0
4	ВЗР	В	401	19/19	0.90	0.14	19,28,40,44	0
7	EDO	В	424	4/4	0.91	0.09	45,45,49,51	0
7	EDO	В	415	4/4	0.95	0.10	35,36,39,40	0
6	ACT	В	403	4/4	0.97	0.07	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.

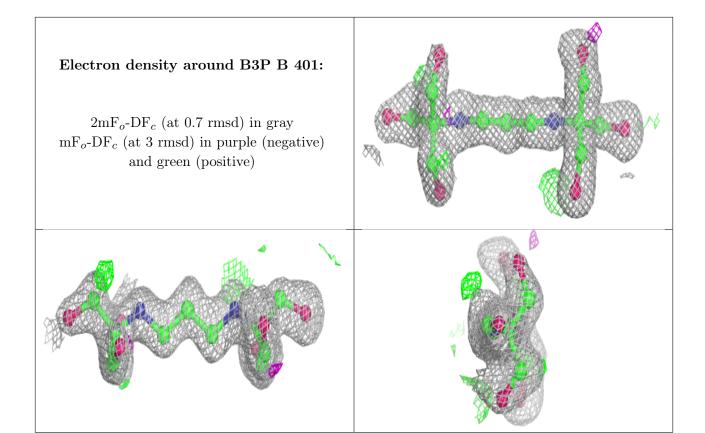


Electron density around ACT B 405: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_{o}\text{-}\mathrm{DF}_{c}$ (at 3 rmsd) in purple (negative) and green (positive)

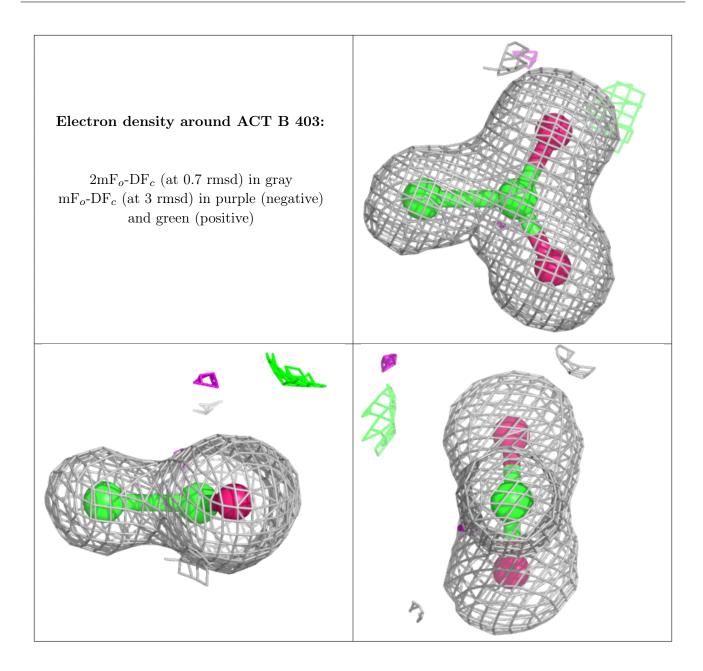












6.5 Other polymers (i)

There are no such residues in this entry.

