



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 PM UTC

PDB ID : 5MI7 / pdb_00005mi7
Title : BtGH84 mutant with covalent modification by MA4 in complex with PUGNAc
Authors : Darby, J.F.; Davies, G.J.; Hubbard, R.E.
Deposited on : 2016-11-27
Resolution : 2.10 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

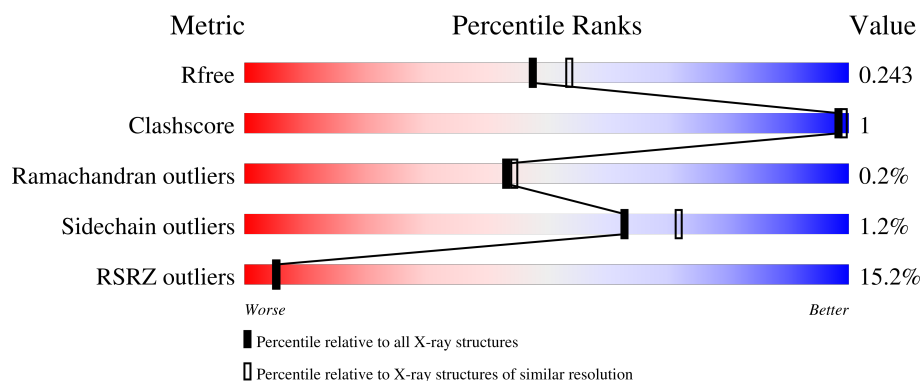
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	A	727	14% 90% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11034 atoms, of which 5400 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.

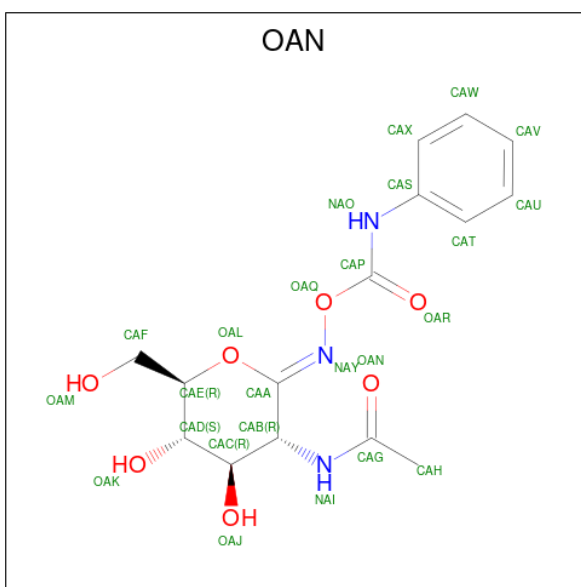
- Molecule 1 is a protein called O-GlcNAcase BT_4395.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	671	Total	C	H	N	O	S	0	0	0
			10815	3485	5368	922	1022	18			

There are 15 discrepancies between the modelled and reference sequences:

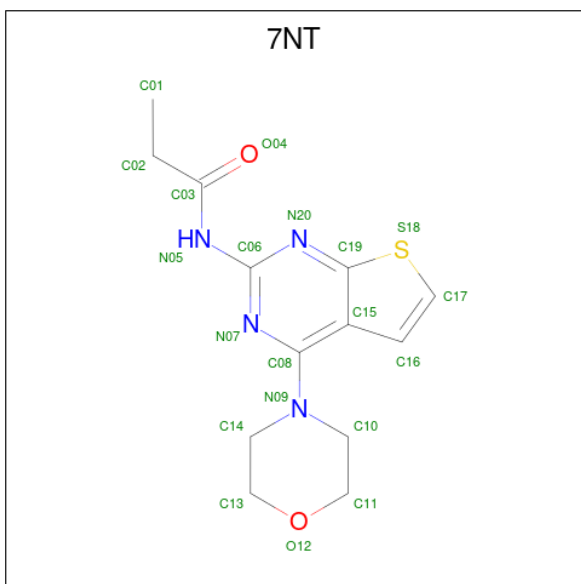
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q89ZI2
A	-9	GLY	-	expression tag	UNP Q89ZI2
A	-8	SER	-	expression tag	UNP Q89ZI2
A	-7	SER	-	expression tag	UNP Q89ZI2
A	-6	HIS	-	expression tag	UNP Q89ZI2
A	-5	HIS	-	expression tag	UNP Q89ZI2
A	-4	HIS	-	expression tag	UNP Q89ZI2
A	-3	HIS	-	expression tag	UNP Q89ZI2
A	-2	HIS	-	expression tag	UNP Q89ZI2
A	-1	HIS	-	expression tag	UNP Q89ZI2
A	0	GLN	-	expression tag	UNP Q89ZI2
A	1	TRP	-	expression tag	UNP Q89ZI2
A	420	SER	CYS	engineered mutation	UNP Q89ZI2
A	550	CYS	TYR	engineered mutation	UNP Q89ZI2
A	654	SER	CYS	engineered mutation	UNP Q89ZI2

- Molecule 2 is O-(2-ACETAMIDO-2-DEOXY D-GLUCOPYRANOSYLIDENE) AMINO-N-PHENYLCARBAMATE (CCD ID: OAN) (formula: C₁₅H₁₉N₃O₇).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			44	15	19	3	7		

- Molecule 3 is {N}-(4-morpholin-4-ylthieno[2,3-d]pyrimidin-2-yl)propanamide (CCD ID: 7NT) (formula: C₁₃H₁₆N₄O₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			33	13	13	4	2	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0

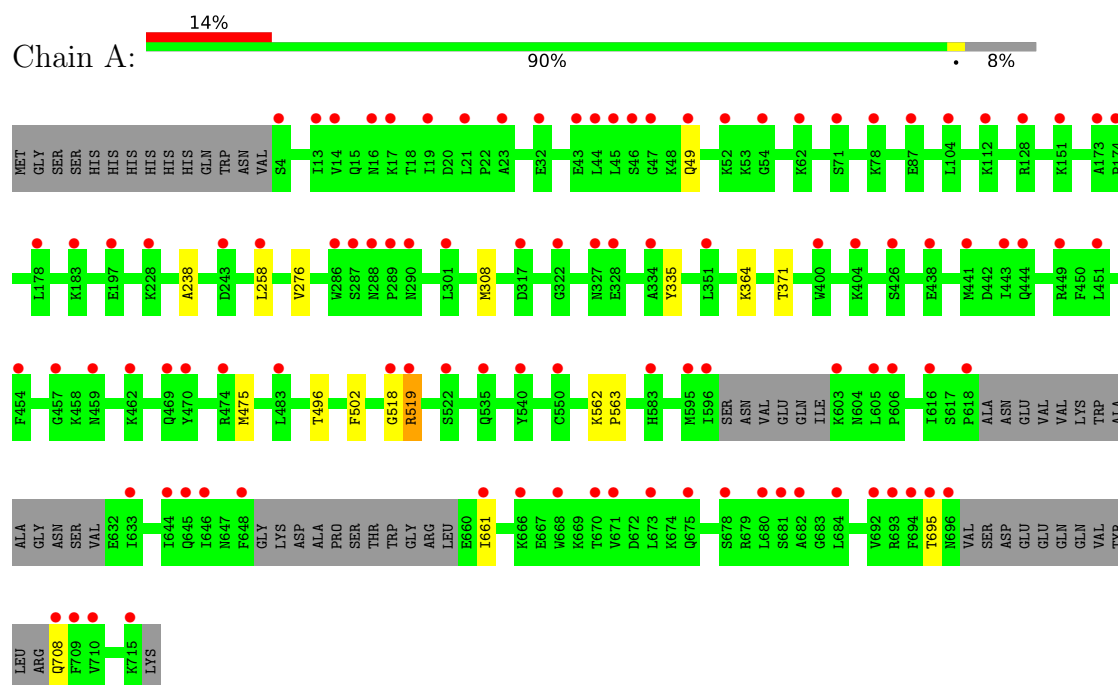
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	141	Total 141	O 141	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: O-GlcNAcase BT_4395



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.19Å 51.82Å 108.23Å 90.00° 111.61° 90.00°	Depositor
Resolution (Å)	100.62 – 2.10 100.62 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (100.62-2.10) 99.4 (100.62-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.213 , 0.249 0.207 , 0.243	Depositor DCC
R_{free} test set	2953 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.814	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11034	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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: 7NT, OAN, CA

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	0.14	0/5580	0.32	0/7555

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	5447	5368	5368	6	0
2	A	25	19	19	0	0
3	A	20	13	0	0	0
4	A	1	0	0	0	0
5	A	141	0	0	1	0
All	All	5634	5400	5387	6	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 1.

All (6) 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:708:GLN:N	5:A:902:HOH:O	2.30	0.63
1:A:238:ALA:HA	1:A:276:VAL:O	2.18	0.44
1:A:308:MET:HA	1:A:335:TYR:O	2.19	0.42
1:A:562:LYS:HB3	1:A:563:PRO:HD3	2.02	0.42
1:A:475:MET:HE3	1:A:502:PHE:CE1	2.55	0.41
1:A:518:GLY:O	1:A:519:ARG:HB2	2.21	0.41

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	661/727 (91%)	631 (96%)	29 (4%)	1 (0%)	43 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	519	ARG

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	A	592/640 (92%)	585 (99%)	7 (1%)	63 72

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	258	LEU
1	A	364	LYS
1	A	371	THR
1	A	496	THR
1	A	661	ILE
1	A	695	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	349	HIS
1	A	425	ASN
1	A	469	GLN

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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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
2	OAN	A	801	-	23,26,26	1.64	2 (8%)	24,35,35	1.67	3 (12%)
3	7NT	A	802	1	22,22,22	2.59	8 (36%)	27,30,30	2.38	13 (48%)

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	OAN	A	801	-	-	3/12/35/35	0/2/2/2
3	7NT	A	802	1	-	2/10/18/18	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	7NT	C19-S18	6.09	1.80	1.73
3	A	802	7NT	C08-N09	5.37	1.50	1.37
2	A	801	OAN	OAQ-NAY	-5.33	1.32	1.44
3	A	802	7NT	C06-N05	4.30	1.44	1.38
2	A	801	OAN	OAL-CAE	-3.74	1.41	1.46
3	A	802	7NT	O04-C03	-3.55	1.16	1.23
3	A	802	7NT	C19-N20	3.08	1.37	1.33
3	A	802	7NT	C03-N05	2.95	1.42	1.35
3	A	802	7NT	C14-N09	2.43	1.50	1.46
3	A	802	7NT	C06-N07	2.40	1.41	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	7NT	C19-S18-C17	5.57	92.27	90.62
2	A	801	OAN	CAS-NAO-CAP	-5.46	117.76	126.39
3	A	802	7NT	S18-C19-N20	3.62	126.72	122.51
3	A	802	7NT	C15-C08-N09	-3.49	117.29	122.81
3	A	802	7NT	C06-N05-C03	-3.46	123.25	129.24
3	A	802	7NT	C19-C15-C16	-3.23	108.88	111.76
3	A	802	7NT	C15-C19-N20	-3.17	124.41	126.55
3	A	802	7NT	C15-C19-S18	-3.11	108.87	111.38
3	A	802	7NT	N20-C06-N07	-3.08	121.21	126.26
3	A	802	7NT	C14-N09-C10	-3.02	104.78	111.57
3	A	802	7NT	N07-C08-N09	2.52	121.52	116.77
2	A	801	OAN	CAX-CAS-CAT	2.46	122.30	119.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	7NT	C02-C03-N05	2.22	120.38	114.65
3	A	802	7NT	C06-N07-C08	2.21	121.08	113.99
2	A	801	OAN	OAJ-CAC-CAB	-2.17	104.60	108.98
3	A	802	7NT	C15-C16-C17	2.04	118.84	111.70

There are no chirality outliers.

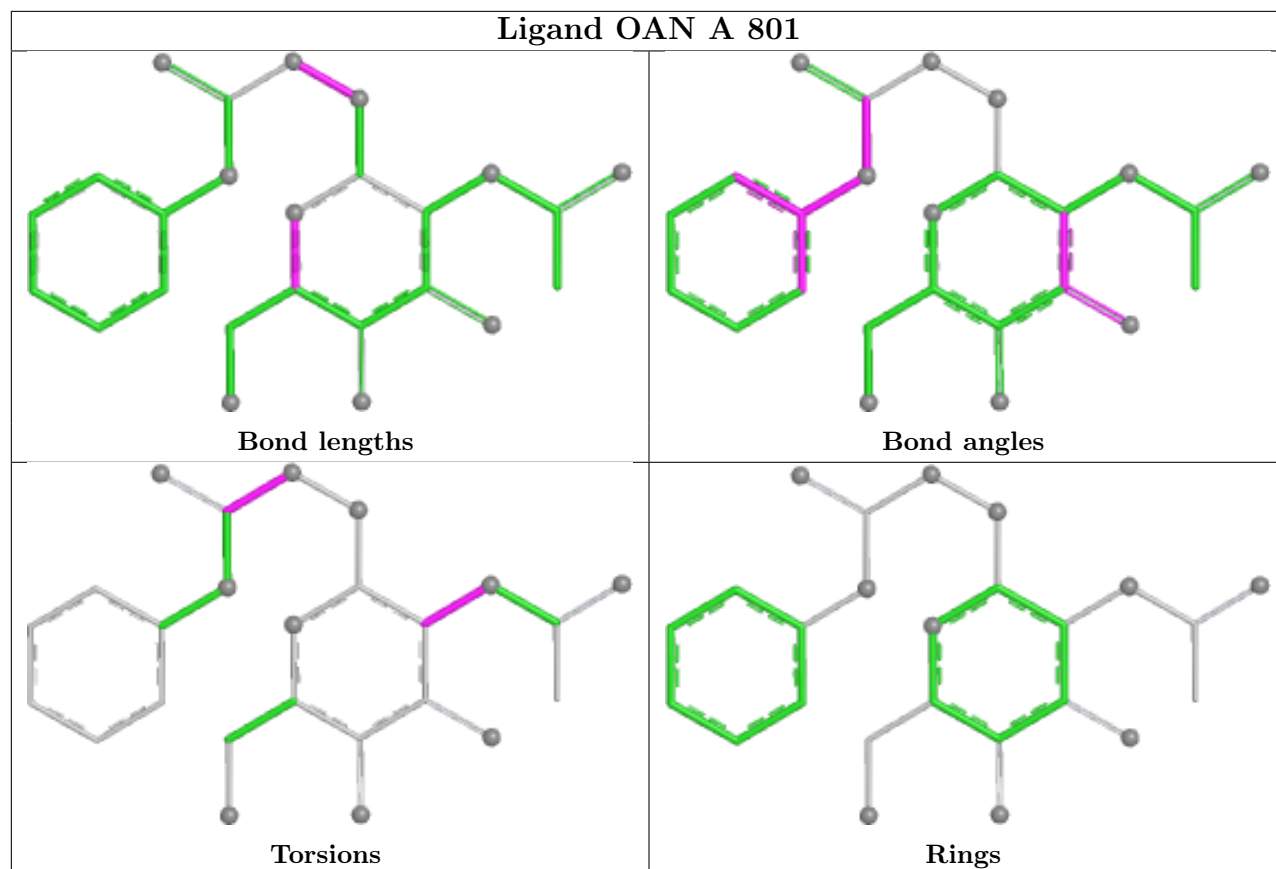
All (5) torsion outliers are listed below:

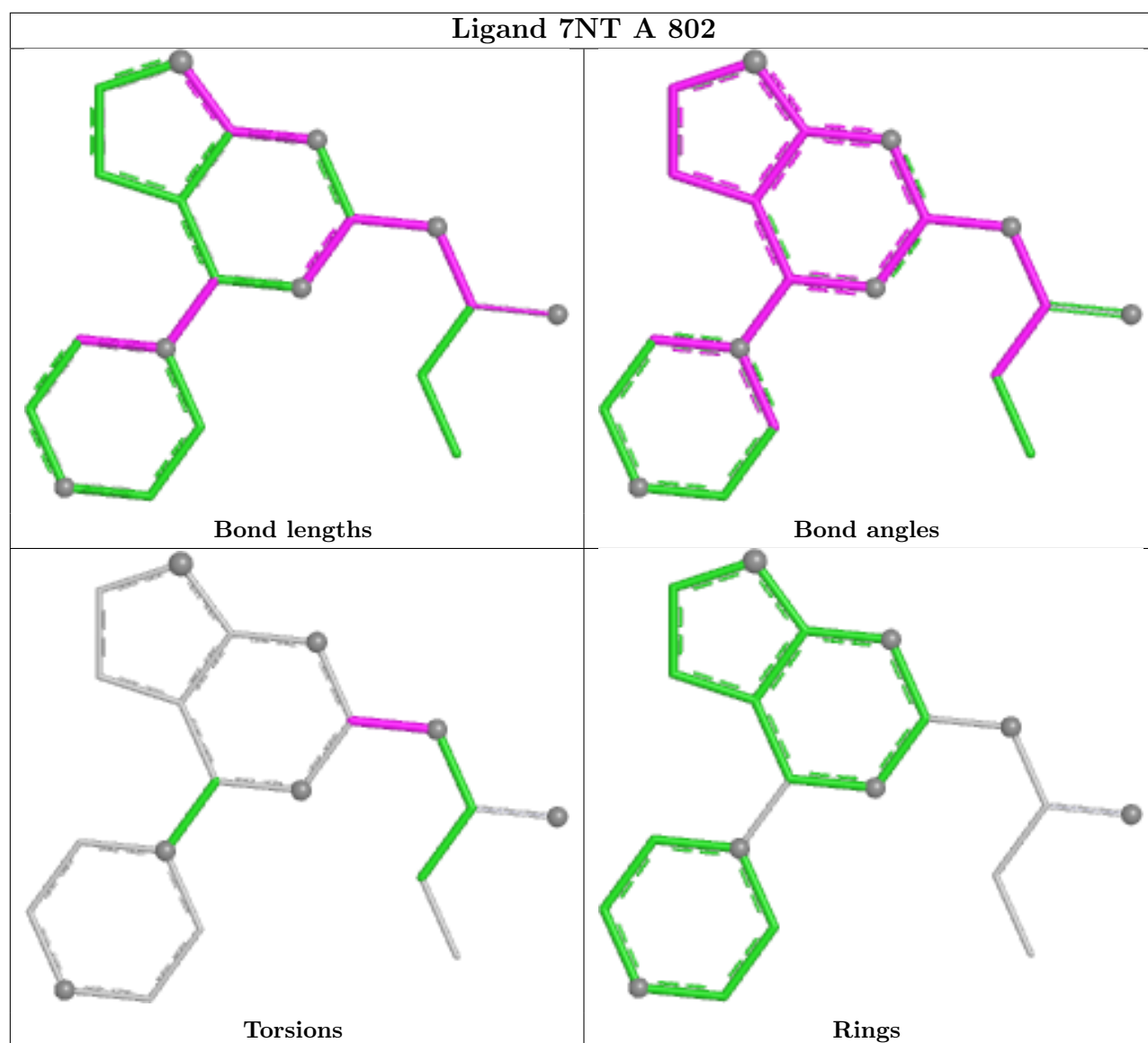
Mol	Chain	Res	Type	Atoms
2	A	801	OAN	OAR-CAP-OAQ-NAY
2	A	801	OAN	NAO-CAP-OAQ-NAY
3	A	802	7NT	N07-C06-N05-C03
3	A	802	7NT	N20-C06-N05-C03
2	A	801	OAN	CAA-CAB-NAI-CAG

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 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 ⓘ

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	A	671/727 (92%)	1.03	102 (15%) 5 5	26, 51, 106, 147	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	694	PHE	6.2
1	A	648	PHE	5.0
1	A	596	ILE	4.9
1	A	696	ASN	4.6
1	A	695	THR	4.4
1	A	519	ARG	4.4
1	A	661	ILE	4.1
1	A	618	PRO	4.0
1	A	462	LYS	3.9
1	A	715	LYS	3.6
1	A	603	LYS	3.6
1	A	633	ILE	3.6
1	A	174	PRO	3.6
1	A	595	MET	3.5
1	A	671	VAL	3.5
1	A	692	VAL	3.5
1	A	16	ASN	3.5
1	A	678	SER	3.4
1	A	605	LEU	3.4
1	A	46	SER	3.3
1	A	644	ILE	3.2
1	A	470	TYR	3.2
1	A	71	SER	3.2
1	A	693	ARG	3.1
1	A	474	ARG	3.1
1	A	483	LEU	3.1
1	A	17	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	673	LEU	3.0
1	A	670	THR	3.0
1	A	459	ASN	2.9
1	A	606	PRO	2.9
1	A	680	LEU	2.9
1	A	668	TRP	2.8
1	A	404	LYS	2.8
1	A	19	ILE	2.8
1	A	666	LYS	2.7
1	A	708	GLN	2.7
1	A	535	GLN	2.6
1	A	287	SER	2.6
1	A	87	GLU	2.5
1	A	286	TRP	2.5
1	A	518	GLY	2.5
1	A	290	ASN	2.5
1	A	550	CYS	2.5
1	A	104	LEU	2.5
1	A	328	GLU	2.4
1	A	682	ALA	2.4
1	A	52	LYS	2.4
1	A	78	LYS	2.4
1	A	183	LYS	2.4
1	A	13	ILE	2.4
1	A	469	GLN	2.4
1	A	173	ALA	2.4
1	A	43	GLU	2.4
1	A	228	LYS	2.4
1	A	289	PRO	2.4
1	A	178	LEU	2.4
1	A	258	LEU	2.4
1	A	443	ILE	2.4
1	A	646	ILE	2.3
1	A	128	ARG	2.3
1	A	616	ILE	2.3
1	A	47	GLY	2.3
1	A	301	LEU	2.3
1	A	62	LYS	2.3
1	A	151	LYS	2.3
1	A	334	ALA	2.3
1	A	540	TYR	2.3
1	A	454	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	112	LYS	2.2
1	A	21	LEU	2.2
1	A	45	LEU	2.2
1	A	351	LEU	2.2
1	A	32	GLU	2.2
1	A	400	TRP	2.2
1	A	444	GLN	2.2
1	A	4	SER	2.2
1	A	522	SER	2.2
1	A	14	VAL	2.2
1	A	457	GLY	2.2
1	A	684	LEU	2.2
1	A	675	GLN	2.2
1	A	288	ASN	2.2
1	A	710	VAL	2.2
1	A	583	HIS	2.2
1	A	681	SER	2.1
1	A	709	PHE	2.1
1	A	54	GLY	2.1
1	A	322	GLY	2.1
1	A	426	SER	2.1
1	A	243	ASP	2.1
1	A	449	ARG	2.1
1	A	451	LEU	2.1
1	A	441	MET	2.1
1	A	327	ASN	2.1
1	A	645	GLN	2.1
1	A	23	ALA	2.1
1	A	49	GLN	2.0
1	A	317	ASP	2.0
1	A	197	GLU	2.0
1	A	438	GLU	2.0
1	A	44	LEU	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](#)

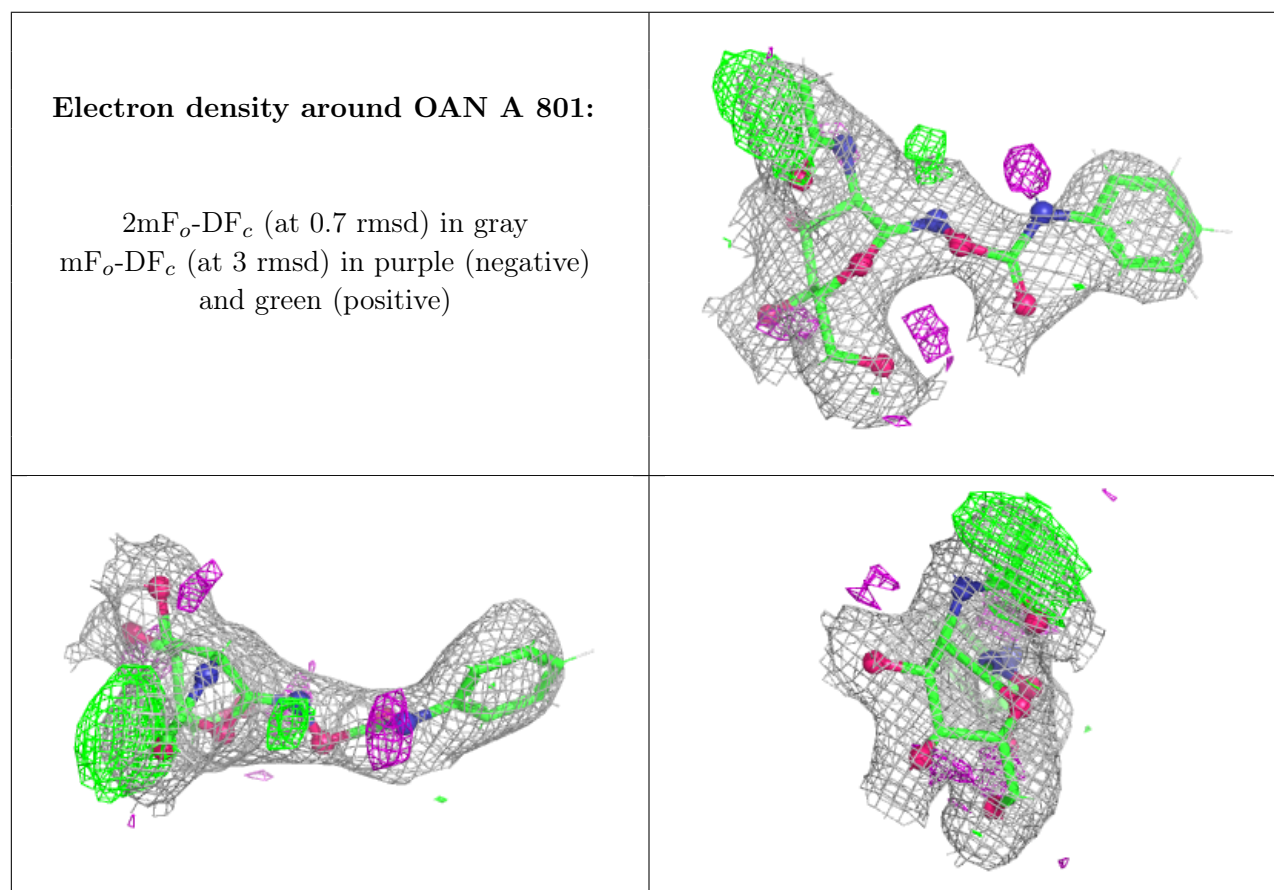
There are no oligosaccharides in this entry.

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.

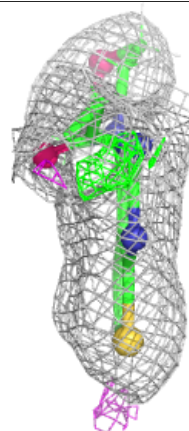
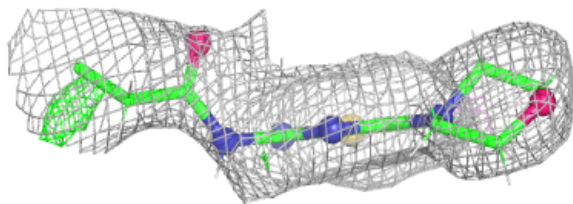
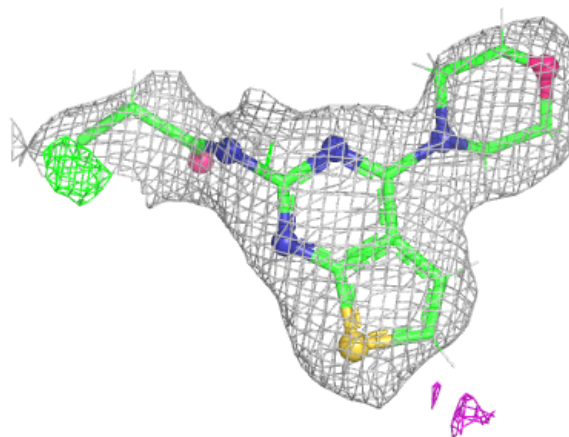
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OAN	A	801	25/25	0.87	0.18	26,54,108,121	0
3	7NT	A	802	20/20	0.90	0.19	70,84,103,117	0
4	CA	A	803	1/1	0.98	0.06	40,40,40,40	0

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 7NT A 802:

$2mF_o-DF_c$ (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.