



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:42 AM UTC

PDB ID : 5MI5 / pdb_00005mi5
Title : BtGH84 mutant with covalent modification by MA3 in complex with PUGNAc
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Deposited on : 2016-11-27
Resolution : 2.15 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

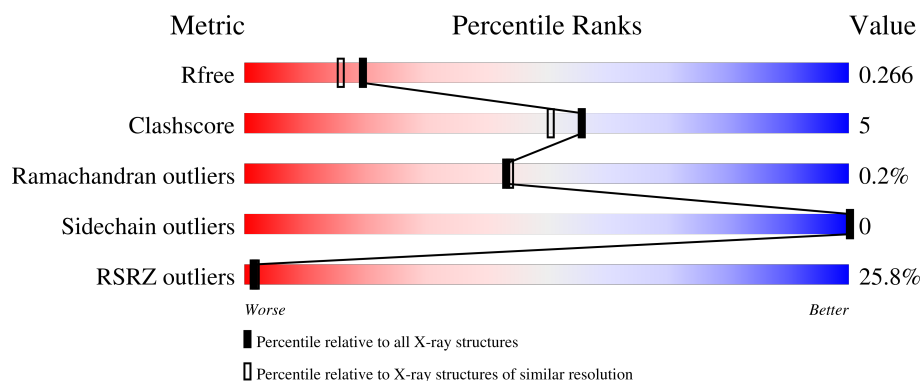
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	24% 85% 8% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5786 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.

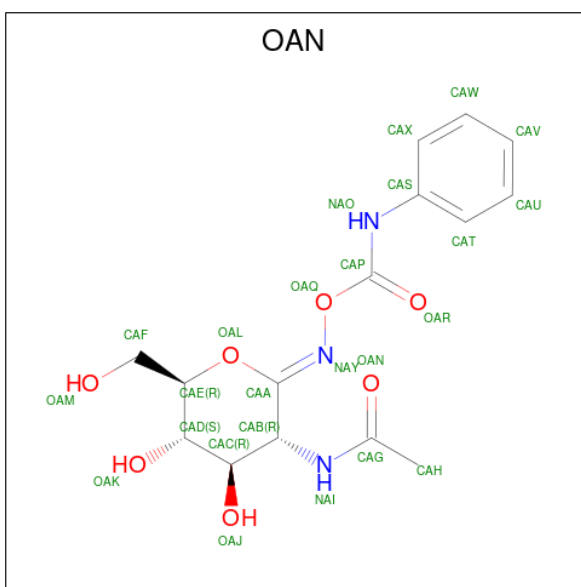
- Molecule 1 is a protein called O-GlcNAcase BT_4395.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	0	1	0
			5490	3510	931	1030	19			

There are 15 discrepancies between the modelled and reference sequences:

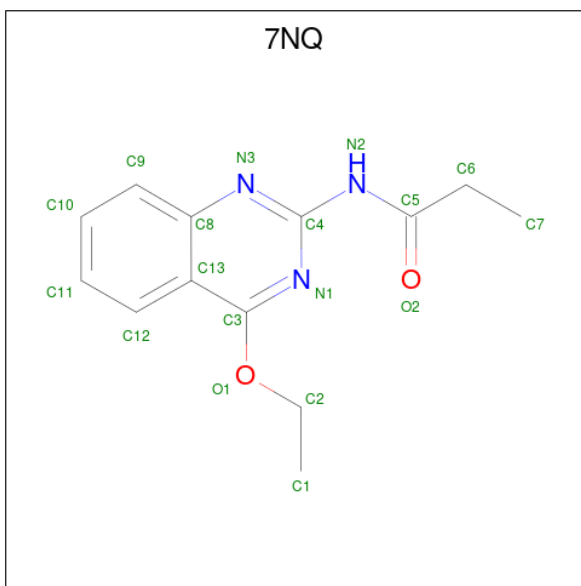
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q89ZI2
A	-9	GLY	-	expression tag	UNP Q89ZI2
A	-8	SER	-	expression tag	UNP Q89ZI2
A	-7	SER	-	expression tag	UNP Q89ZI2
A	-6	HIS	-	expression tag	UNP Q89ZI2
A	-5	HIS	-	expression tag	UNP Q89ZI2
A	-4	HIS	-	expression tag	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	N	O	0	0
			25	15	3	7		

- Molecule 3 is {N}-(4-ethoxyquinazolin-2-yl)propanamide (CCD ID: 7NQ) (formula: $C_{13}H_{15}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	13	3	2		

- 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	252	Total 252	O 252	0	0

- 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	198.22Å 52.12Å 112.78Å 90.00° 113.24° 90.00°	Depositor
Resolution (Å)	51.81 – 2.15 51.81 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.2 (51.81-2.15) 99.7 (51.81-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.233 , 0.272 0.226 , 0.266	Depositor DCC
R_{free} test set	2913 reflections (1.79%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5786	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: OAN, 7NQ, 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	0.18	0/5623	0.37	0/7607

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	5490	0	5412	51	0
2	A	25	0	19	0	0
3	A	18	0	0	0	0
4	A	1	0	0	0	0
5	A	252	0	0	8	1
All	All	5786	0	5431	51	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 5.

All (51) 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:448:GLU:HB3	1:A:452:LYS:NZ	1.71	1.05
1:A:448:GLU:HB3	1:A:452:LYS:HZ3	0.93	1.05
1:A:448:GLU:O	1:A:452:LYS:HD3	1.64	0.96
1:A:448:GLU:CB	1:A:452:LYS:HZ3	1.80	0.95
1:A:442:ASP:OD2	5:A:901:HOH:O	1.87	0.93
1:A:483:LEU:HD23	1:A:484:MET:CE	2.06	0.84
1:A:483:LEU:HD23	1:A:484:MET:HE3	1.60	0.83
1:A:6:GLN:H	1:A:109:GLN:HE22	1.30	0.78
1:A:318:ILE:H	1:A:358:ASN:HD22	1.33	0.76
1:A:448:GLU:CB	1:A:452:LYS:NZ	2.44	0.75
1:A:693:ARG:NH2	5:A:902:HOH:O	2.11	0.75
1:A:660:GLU:OE2	1:A:693:ARG:NH2	2.23	0.72
1:A:52:LYS:O	1:A:52:LYS:NZ	2.24	0.70
1:A:603:LYS:HD3	1:A:605:LEU:HD23	1.72	0.70
1:A:673:LEU:HD23	1:A:680:LEU:HB3	1.80	0.62
1:A:318:ILE:H	1:A:358:ASN:ND2	1.98	0.61
1:A:698:SER:OG	1:A:699:ASP:N	2.34	0.60
1:A:260:TYR:CZ	1:A:264:LYS:HD3	2.38	0.59
1:A:693:ARG:HD3	1:A:695:THR:OG1	2.02	0.59
1:A:555:LYS:NZ	5:A:914:HOH:O	2.36	0.58
1:A:483:LEU:HD23	1:A:484:MET:HE2	1.84	0.58
1:A:260:TYR:CE1	1:A:264:LYS:HD3	2.40	0.56
1:A:659:LEU:HD12	5:A:902:HOH:O	2.04	0.56
1:A:693:ARG:HD2	1:A:694:PHE:N	2.22	0.55
1:A:483:LEU:CD2	1:A:484:MET:HE3	2.36	0.52
1:A:660:GLU:OE2	1:A:693:ARG:CZ	2.59	0.50
1:A:424:HIS:HE1	5:A:901:HOH:O	1.95	0.50
1:A:660:GLU:OE2	1:A:693:ARG:NH1	2.45	0.49
1:A:4:SER:N	5:A:923:HOH:O	2.45	0.48
1:A:417:GLU:OE2	1:A:417:GLU:N	2.37	0.48
1:A:289:PRO:O	5:A:903:HOH:O	2.20	0.47
1:A:291:GLY:O	5:A:903:HOH:O	2.20	0.47
1:A:33:ALA:HB2	1:A:60:GLY:HA2	1.96	0.46
1:A:630:SER:O	1:A:632:GLU:N	2.49	0.46
1:A:471:THR:O	1:A:475:MET:HG3	2.15	0.46
1:A:326:ILE:O	1:A:330:ILE:HG12	2.15	0.46
1:A:475:MET:HE3	1:A:502:PHE:CE1	2.51	0.46
1:A:557:ALA:HB1	1:A:561:ILE:HB	1.99	0.45
1:A:456:GLU:HG3	1:A:458:LYS:HD2	1.99	0.45
1:A:603:LYS:HB3	1:A:603:LYS:HE2	1.76	0.44
1:A:519:ARG:H	1:A:519:ARG:HG2	1.59	0.44
1:A:695:THR:HG22	1:A:697:VAL:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ALA:HA	1:A:276:VAL:O	2.18	0.43
1:A:81:TYR:HA	1:A:94:GLY:HA2	2.01	0.42
1:A:59:ILE:HA	1:A:92:LEU:O	2.20	0.42
1:A:158:MET:HE1	1:A:384:ILE:HG23	2.03	0.41
1:A:692:VAL:HG21	1:A:711:LEU:HD22	2.01	0.41
1:A:340:PHE:CD1	1:A:341:PRO:HA	2.55	0.41
1:A:292:ASN:OD1	1:A:292:ASN:N	2.54	0.41
1:A:340:PHE:O	1:A:371:THR:OG1	2.31	0.40
1:A:348:ASP:OD1	1:A:348:ASP:N	2.53	0.40

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)
5:A:959:HOH:O	5:A:959:HOH:O[2_555]	1.90	0.30

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	662/727 (91%)	630 (95%)	31 (5%)	1 (0%)	43 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	518	GLY

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	597/640 (93%)	597 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	109	GLN
1	A	187	GLN
1	A	349	HIS
1	A	358	ASN
1	A	393	ASN
1	A	536	GLN
1	A	547	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	1.57	2 (8%)	24,35,35	1.80	5 (20%)
3	7NQ	A	802	1	19,19,19	2.17	5 (26%)	25,25,25	2.82	11 (44%)

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	-	-	4/12/35/35	0/2/2/2
3	7NQ	A	802	1	-	4/9/9/9	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	7NQ	C4-N2	4.79	1.45	1.38
2	A	801	OAN	OAQ-NAY	-4.68	1.33	1.44
3	A	802	7NQ	C5-N2	4.53	1.45	1.35
3	A	802	7NQ	O1-C3	4.42	1.40	1.34
3	A	802	7NQ	C13-C8	-3.68	1.36	1.42
2	A	801	OAN	OAL-CAE	-3.68	1.41	1.46
3	A	802	7NQ	O2-C5	-2.11	1.19	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	7NQ	C4-N2-C5	-7.43	116.40	129.24
2	A	801	OAN	CAS-NAO-CAP	-5.49	117.70	126.39
3	A	802	7NQ	C3-C13-C8	5.31	118.27	114.77
3	A	802	7NQ	C13-C3-N1	-5.07	119.50	124.68
3	A	802	7NQ	O1-C3-C13	4.66	119.93	115.01
2	A	801	OAN	CAC-CAD-CAE	-3.95	103.07	110.23
3	A	802	7NQ	C13-C8-N3	-3.55	119.04	122.80
3	A	802	7NQ	C4-N3-C8	3.45	121.01	115.54
3	A	802	7NQ	C4-N1-C3	3.03	120.54	115.38
3	A	802	7NQ	N3-C4-N1	-2.82	121.64	126.25
2	A	801	OAN	CAX-CAS-CAT	2.36	122.17	119.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	OAN	OAK-CAD-CAC	-2.29	104.97	110.38
3	A	802	7NQ	C6-C5-N2	2.25	120.45	114.65
3	A	802	7NQ	C2-O1-C3	-2.18	114.51	117.32
2	A	801	OAN	OAJ-CAC-CAB	-2.14	104.64	108.98
3	A	802	7NQ	O2-C5-N2	-2.10	119.87	123.64

There are no chirality outliers.

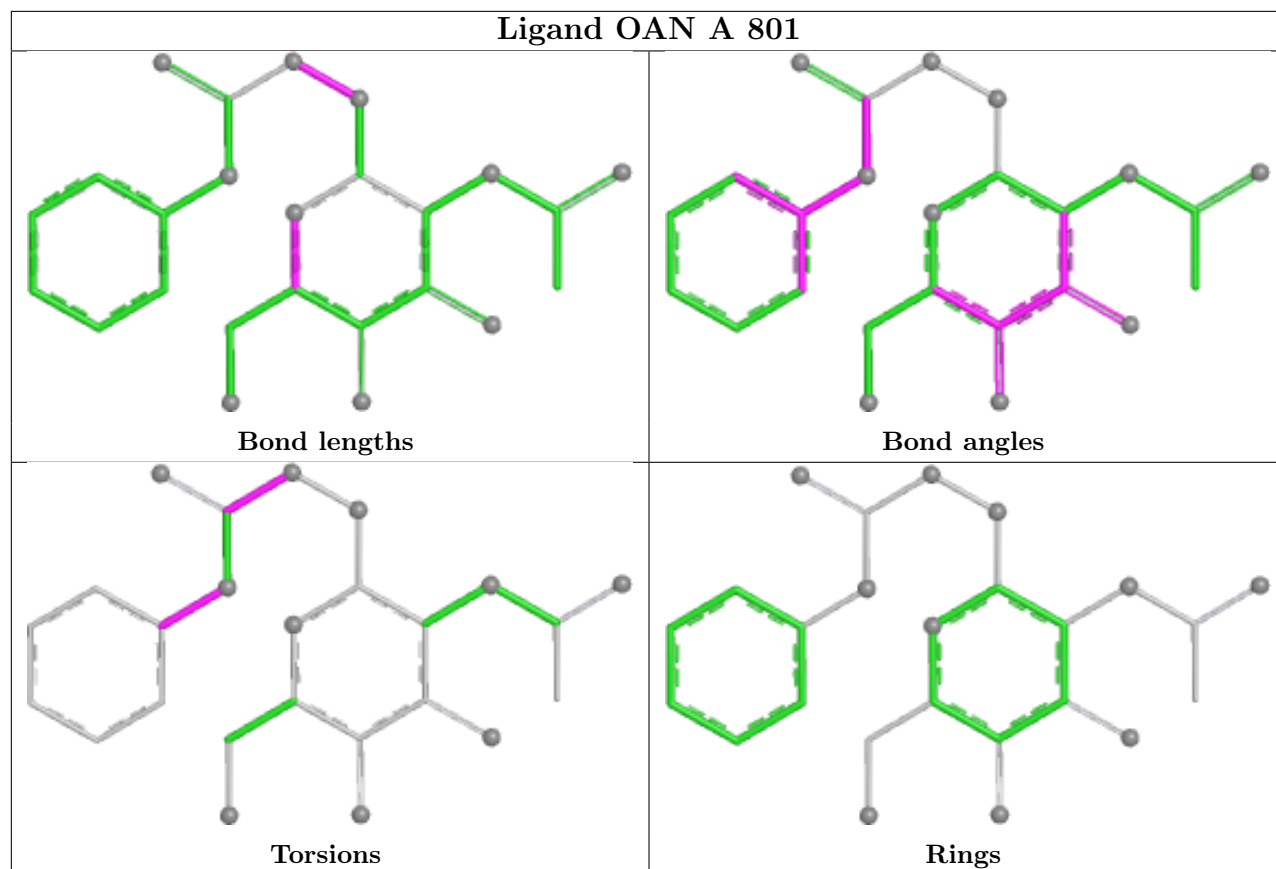
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	OAN	OAR-CAP-OAQ-NAY
2	A	801	OAN	NAO-CAP-OAQ-NAY
3	A	802	7NQ	N1-C4-N2-C5
3	A	802	7NQ	N3-C4-N2-C5
3	A	802	7NQ	C13-C3-O1-C2
2	A	801	OAN	CAT-CAS-NAO-CAP
2	A	801	OAN	CAX-CAS-NAO-CAP
3	A	802	7NQ	N1-C3-O1-C2

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	677/727 (93%)	1.64	175 (25%) 1 2	24, 43, 94, 123	1 (0%)

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	659	LEU	9.1
1	A	619	ALA	7.9
1	A	697	VAL	7.6
1	A	671	VAL	6.0
1	A	628	GLY	5.4
1	A	707	ARG	5.2
1	A	4	SER	5.1
1	A	630	SER	4.8
1	A	286	TRP	4.8
1	A	682	ALA	4.8
1	A	540	TYR	4.7
1	A	483	LEU	4.7
1	A	52	LYS	4.7
1	A	519	ARG	4.6
1	A	605	LEU	4.6
1	A	23	ALA	4.6
1	A	595	MET	4.4
1	A	693	ARG	4.3
1	A	648	PHE	4.2
1	A	698	SER	4.1
1	A	454	PHE	4.0
1	A	604	ASN	4.0
1	A	670	THR	4.0
1	A	618	PRO	3.9
1	A	680	LEU	3.9
1	A	53	LYS	3.9
1	A	629	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	452	LYS	3.8
1	A	695	THR	3.8
1	A	287	SER	3.7
1	A	683	GLY	3.7
1	A	679	ARG	3.7
1	A	518	GLY	3.7
1	A	694	PHE	3.7
1	A	646	ILE	3.6
1	A	678	SER	3.6
1	A	21	LEU	3.6
1	A	15	GLN	3.6
1	A	400	TRP	3.5
1	A	47	GLY	3.5
1	A	666	LYS	3.4
1	A	715	LYS	3.4
1	A	672	ASP	3.4
1	A	603	LYS	3.4
1	A	334	ALA	3.4
1	A	616	ILE	3.4
1	A	45	LEU	3.4
1	A	16	ASN	3.3
1	A	457	GLY	3.2
1	A	470	TYR	3.2
1	A	25	TYR	3.2
1	A	647	ASN	3.2
1	A	673	LEU	3.2
1	A	699	ASP	3.2
1	A	606	PRO	3.2
1	A	550	CYS	3.2
1	A	668	TRP	3.1
1	A	456	GLU	3.1
1	A	285	SER	3.1
1	A	244	ILE	3.1
1	A	676	LYS	3.1
1	A	710	VAL	3.1
1	A	295	THR	3.1
1	A	675	GLN	3.1
1	A	709	PHE	3.1
1	A	669	LYS	3.1
1	A	111	LEU	3.0
1	A	24	VAL	3.0
1	A	51	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	451	LEU	3.0
1	A	442	ASP	2.9
1	A	615	LEU	2.9
1	A	323	ILE	2.9
1	A	72	ARG	2.9
1	A	17	LYS	2.9
1	A	213	LYS	2.9
1	A	328	GLU	2.8
1	A	216	LYS	2.8
1	A	594	LYS	2.8
1	A	692	VAL	2.8
1	A	290	ASN	2.8
1	A	246	GLY	2.8
1	A	458	LYS	2.8
1	A	55	MET	2.8
1	A	661	ILE	2.8
1	A	643	ASN	2.7
1	A	538	MET	2.7
1	A	289	PRO	2.7
1	A	268	VAL	2.7
1	A	43	GLU	2.7
1	A	441	MET	2.7
1	A	644	ILE	2.7
1	A	337	TRP	2.7
1	A	54	GLY	2.7
1	A	463	ALA	2.7
1	A	188	LEU	2.7
1	A	396	LYS	2.7
1	A	118	GLU	2.6
1	A	459	ASN	2.6
1	A	13	ILE	2.6
1	A	14	VAL	2.6
1	A	633	ILE	2.6
1	A	88	LYS	2.6
1	A	321	ASP	2.6
1	A	387	VAL	2.5
1	A	103	ALA	2.5
1	A	583	HIS	2.5
1	A	681	SER	2.5
1	A	22	PRO	2.5
1	A	277	MET	2.4
1	A	455	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	128	ARG	2.4
1	A	377	ALA	2.4
1	A	687	ALA	2.4
1	A	443	ILE	2.3
1	A	303	PRO	2.3
1	A	264	LYS	2.3
1	A	561	ILE	2.3
1	A	292	ASN	2.3
1	A	297	LEU	2.3
1	A	428	LEU	2.3
1	A	435	TYR	2.3
1	A	307	ILE	2.3
1	A	663	THR	2.3
1	A	317	ASP	2.3
1	A	221	LEU	2.3
1	A	327	ASN	2.2
1	A	11	GLN	2.2
1	A	136	PHE	2.2
1	A	19	ILE	2.2
1	A	331	LYS	2.2
1	A	571	THR	2.2
1	A	172	SER	2.2
1	A	541	ILE	2.2
1	A	689	VAL	2.2
1	A	89	GLU	2.2
1	A	120	GLU	2.2
1	A	138	GLY	2.2
1	A	56	LEU	2.2
1	A	46	SER	2.2
1	A	324	SER	2.2
1	A	343	SER	2.2
1	A	31	GLU	2.1
1	A	632	GLU	2.1
1	A	586	ALA	2.1
1	A	41	LEU	2.1
1	A	423[A]	MET	2.1
1	A	556	THR	2.1
1	A	212	ILE	2.1
1	A	192	VAL	2.1
1	A	570	ALA	2.1
1	A	42	LYS	2.1
1	A	50	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	684	LEU	2.1
1	A	70	TYR	2.1
1	A	154	GLY	2.1
1	A	241	PHE	2.1
1	A	392	TRP	2.1
1	A	112	LYS	2.1
1	A	667	GLU	2.1
1	A	399	THR	2.1
1	A	492	ILE	2.1
1	A	674	LYS	2.1
1	A	403	TRP	2.1
1	A	375	GLU	2.0
1	A	484	MET	2.0
1	A	223	LEU	2.0
1	A	49	GLN	2.0
1	A	708	GLN	2.0
1	A	489	LYS	2.0
1	A	531	VAL	2.0
1	A	389	SER	2.0
1	A	173	ALA	2.0
1	A	214	TRP	2.0
1	A	607	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.

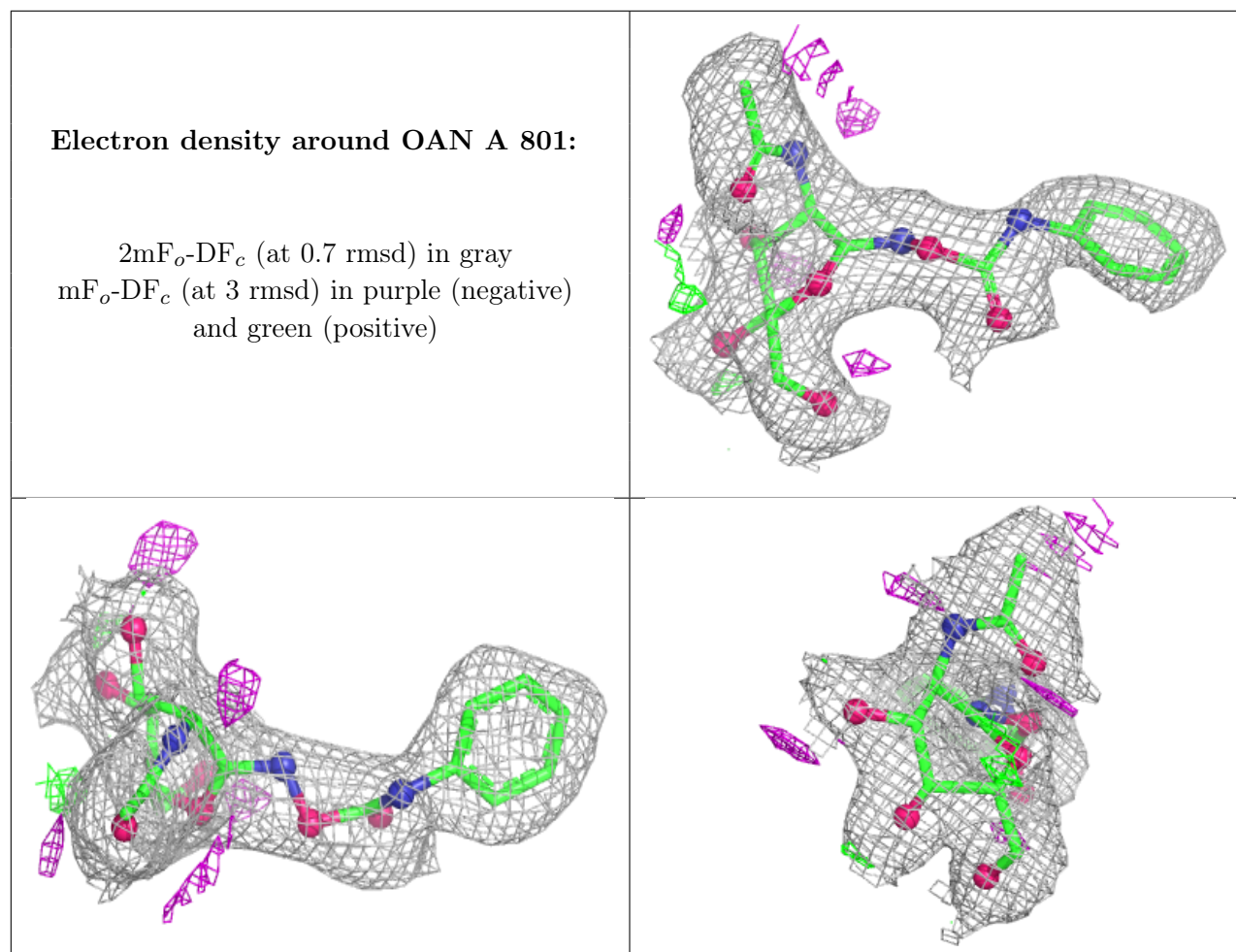
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	7NQ	A	802	18/18	0.89	0.12	36,46,60,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	OAN	A	801	25/25	0.91	0.15	29,44,72,73	0
4	CA	A	803	1/1	0.97	0.18	57,57,57,57	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.