



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2022 – 06:39 pm GMT

PDB ID : 7NG1  
Title : Crystal structure of alpha Carbonic anhydrase from Schistosoma mansoni bound to 1-(4-iodophenyl)-3-[2-(4-sulfamoylphenyl)ethyl]selenourea  
Authors : Ferraroni, M.; Angeli, A.; Supuran, C.T.  
Deposited on : 2021-02-08  
Resolution : 1.67 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.26  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

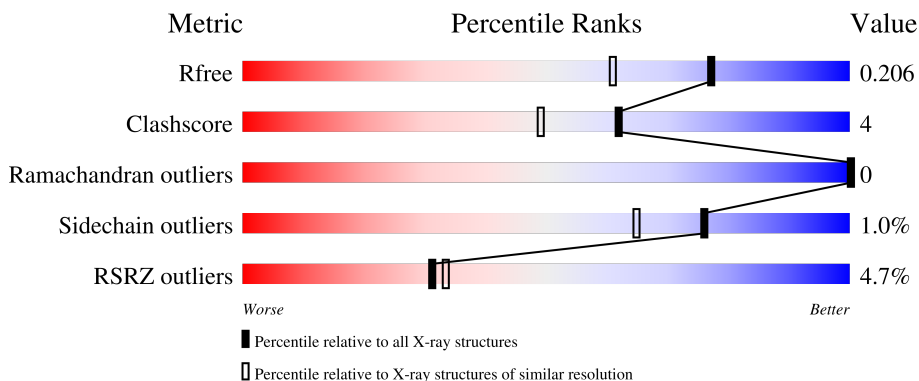
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 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))
$R_{free}$	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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  $\geq 3$ , 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	332	 2% 78% 5% 17%
1	B	332	 5% 78% 6% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	403	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5067 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 Carbonic anhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	277	Total	C	N	O	S	0	2	0
			2243	1432	380	424	7			
1	B	277	Total	C	N	O	S	0	1	0
			2248	1435	385	420	8			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP A0A3Q0KSG2
A	-7	GLU	-	expression tag	UNP A0A3Q0KSG2
A	-6	THR	-	expression tag	UNP A0A3Q0KSG2
A	-5	ASP	-	expression tag	UNP A0A3Q0KSG2
A	-4	THR	-	expression tag	UNP A0A3Q0KSG2
A	-3	LEU	-	expression tag	UNP A0A3Q0KSG2
A	-2	LEU	-	expression tag	UNP A0A3Q0KSG2
A	-1	LEU	-	expression tag	UNP A0A3Q0KSG2
A	0	TRP	-	expression tag	UNP A0A3Q0KSG2
A	1	VAL	-	expression tag	UNP A0A3Q0KSG2
A	2	LEU	-	expression tag	UNP A0A3Q0KSG2
A	3	LEU	-	expression tag	UNP A0A3Q0KSG2
A	4	LEU	-	expression tag	UNP A0A3Q0KSG2
A	5	TRP	-	expression tag	UNP A0A3Q0KSG2
A	6	VAL	-	expression tag	UNP A0A3Q0KSG2
A	7	PRO	-	expression tag	UNP A0A3Q0KSG2
A	8	GLY	-	expression tag	UNP A0A3Q0KSG2
A	9	SER	-	expression tag	UNP A0A3Q0KSG2
A	10	THR	-	expression tag	UNP A0A3Q0KSG2
A	11	GLY	-	expression tag	UNP A0A3Q0KSG2
A	12	ASP	-	expression tag	UNP A0A3Q0KSG2
A	13	ALA	-	expression tag	UNP A0A3Q0KSG2
A	14	ALA	-	expression tag	UNP A0A3Q0KSG2
A	15	GLN	-	expression tag	UNP A0A3Q0KSG2
A	16	PRO	-	expression tag	UNP A0A3Q0KSG2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	17	ALA	-	expression tag	UNP A0A3Q0KSG2
A	18	ARG	-	expression tag	UNP A0A3Q0KSG2
A	19	ARG	-	expression tag	UNP A0A3Q0KSG2
A	20	ALA	-	expression tag	UNP A0A3Q0KSG2
A	299	ARG	-	expression tag	UNP A0A3Q0KSG2
A	300	GLY	-	expression tag	UNP A0A3Q0KSG2
A	301	GLY	-	expression tag	UNP A0A3Q0KSG2
A	302	PRO	-	expression tag	UNP A0A3Q0KSG2
A	303	GLU	-	expression tag	UNP A0A3Q0KSG2
A	304	GLN	-	expression tag	UNP A0A3Q0KSG2
A	305	LYS	-	expression tag	UNP A0A3Q0KSG2
A	306	LEU	-	expression tag	UNP A0A3Q0KSG2
A	307	ILE	-	expression tag	UNP A0A3Q0KSG2
A	308	SER	-	expression tag	UNP A0A3Q0KSG2
A	309	GLU	-	expression tag	UNP A0A3Q0KSG2
A	310	GLU	-	expression tag	UNP A0A3Q0KSG2
A	311	ASP	-	expression tag	UNP A0A3Q0KSG2
A	312	LEU	-	expression tag	UNP A0A3Q0KSG2
A	313	ASN	-	expression tag	UNP A0A3Q0KSG2
A	314	SER	-	expression tag	UNP A0A3Q0KSG2
A	315	ALA	-	expression tag	UNP A0A3Q0KSG2
A	316	VAL	-	expression tag	UNP A0A3Q0KSG2
A	317	ASP	-	expression tag	UNP A0A3Q0KSG2
A	318	HIS	-	expression tag	UNP A0A3Q0KSG2
A	319	HIS	-	expression tag	UNP A0A3Q0KSG2
A	320	HIS	-	expression tag	UNP A0A3Q0KSG2
A	321	HIS	-	expression tag	UNP A0A3Q0KSG2
A	322	HIS	-	expression tag	UNP A0A3Q0KSG2
A	323	HIS	-	expression tag	UNP A0A3Q0KSG2
B	-8	MET	-	initiating methionine	UNP A0A3Q0KSG2
B	-7	GLU	-	expression tag	UNP A0A3Q0KSG2
B	-6	THR	-	expression tag	UNP A0A3Q0KSG2
B	-5	ASP	-	expression tag	UNP A0A3Q0KSG2
B	-4	THR	-	expression tag	UNP A0A3Q0KSG2
B	-3	LEU	-	expression tag	UNP A0A3Q0KSG2
B	-2	LEU	-	expression tag	UNP A0A3Q0KSG2
B	-1	LEU	-	expression tag	UNP A0A3Q0KSG2
B	0	TRP	-	expression tag	UNP A0A3Q0KSG2
B	1	VAL	-	expression tag	UNP A0A3Q0KSG2
B	2	LEU	-	expression tag	UNP A0A3Q0KSG2
B	3	LEU	-	expression tag	UNP A0A3Q0KSG2
B	4	LEU	-	expression tag	UNP A0A3Q0KSG2

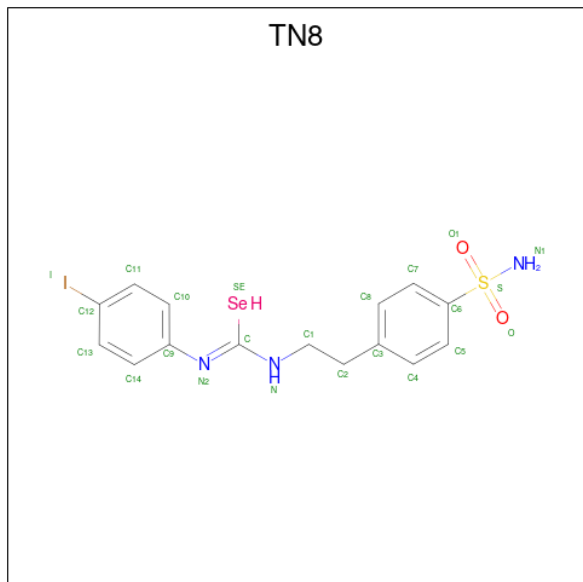
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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	TRP	-	expression tag	UNP A0A3Q0KSG2
B	6	VAL	-	expression tag	UNP A0A3Q0KSG2
B	7	PRO	-	expression tag	UNP A0A3Q0KSG2
B	8	GLY	-	expression tag	UNP A0A3Q0KSG2
B	9	SER	-	expression tag	UNP A0A3Q0KSG2
B	10	THR	-	expression tag	UNP A0A3Q0KSG2
B	11	GLY	-	expression tag	UNP A0A3Q0KSG2
B	12	ASP	-	expression tag	UNP A0A3Q0KSG2
B	13	ALA	-	expression tag	UNP A0A3Q0KSG2
B	14	ALA	-	expression tag	UNP A0A3Q0KSG2
B	15	GLN	-	expression tag	UNP A0A3Q0KSG2
B	16	PRO	-	expression tag	UNP A0A3Q0KSG2
B	17	ALA	-	expression tag	UNP A0A3Q0KSG2
B	18	ARG	-	expression tag	UNP A0A3Q0KSG2
B	19	ARG	-	expression tag	UNP A0A3Q0KSG2
B	20	ALA	-	expression tag	UNP A0A3Q0KSG2
B	299	ARG	-	expression tag	UNP A0A3Q0KSG2
B	300	GLY	-	expression tag	UNP A0A3Q0KSG2
B	301	GLY	-	expression tag	UNP A0A3Q0KSG2
B	302	PRO	-	expression tag	UNP A0A3Q0KSG2
B	303	GLU	-	expression tag	UNP A0A3Q0KSG2
B	304	GLN	-	expression tag	UNP A0A3Q0KSG2
B	305	LYS	-	expression tag	UNP A0A3Q0KSG2
B	306	LEU	-	expression tag	UNP A0A3Q0KSG2
B	307	ILE	-	expression tag	UNP A0A3Q0KSG2
B	308	SER	-	expression tag	UNP A0A3Q0KSG2
B	309	GLU	-	expression tag	UNP A0A3Q0KSG2
B	310	GLU	-	expression tag	UNP A0A3Q0KSG2
B	311	ASP	-	expression tag	UNP A0A3Q0KSG2
B	312	LEU	-	expression tag	UNP A0A3Q0KSG2
B	313	ASN	-	expression tag	UNP A0A3Q0KSG2
B	314	SER	-	expression tag	UNP A0A3Q0KSG2
B	315	ALA	-	expression tag	UNP A0A3Q0KSG2
B	316	VAL	-	expression tag	UNP A0A3Q0KSG2
B	317	ASP	-	expression tag	UNP A0A3Q0KSG2
B	318	HIS	-	expression tag	UNP A0A3Q0KSG2
B	319	HIS	-	expression tag	UNP A0A3Q0KSG2
B	320	HIS	-	expression tag	UNP A0A3Q0KSG2
B	321	HIS	-	expression tag	UNP A0A3Q0KSG2
B	322	HIS	-	expression tag	UNP A0A3Q0KSG2
B	323	HIS	-	expression tag	UNP A0A3Q0KSG2

- Molecule 2 is {N}'-(4-iodophenyl)- {N}]-[2-(4-sulfamoylphenyl)ethyl]carbamimidoselenoi

c acid (three-letter code: TN8) (formula: C<sub>15</sub>H<sub>16</sub>IN<sub>3</sub>O<sub>2</sub>SSe) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
			Total	C	I	N	O	S			Se
2	A	1	23	15	1	3	2	1	1	0	0
2	B	1	23	15	1	3	2	1	1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

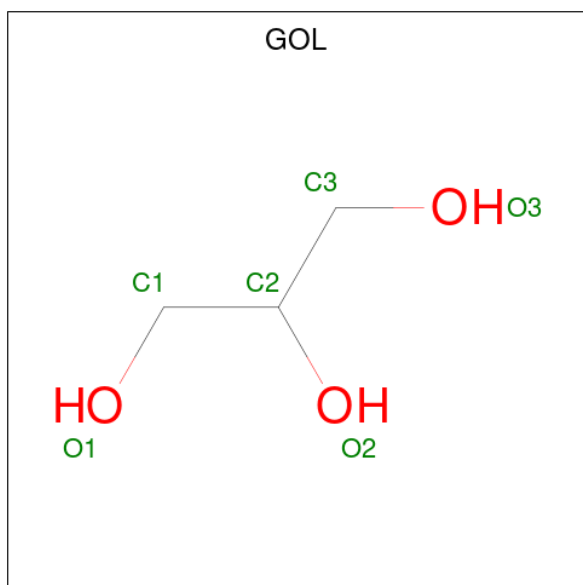
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

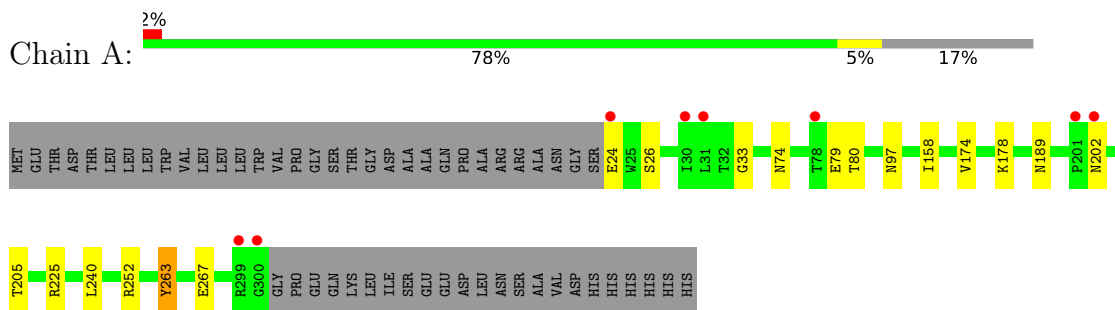
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	248	Total	O	0	0
			248	248		
6	B	218	Total	O	0	0
			218	218		

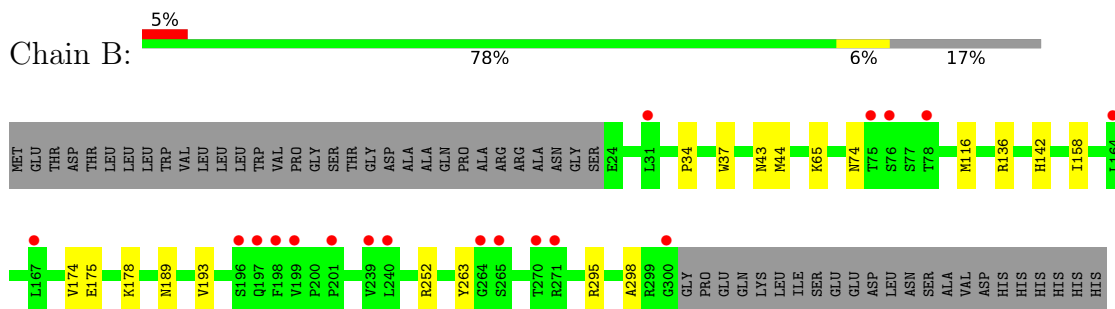
### 3 Residue-property plots [i](#)

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: Carbonic anhydrase



- Molecule 1: Carbonic anhydrase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.28Å 103.28Å 132.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.67 48.13 – 1.67	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-1.67) 100.0 (48.13-1.67)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 1.67Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.178 , 0.205 0.178 , 0.206	Depositor DCC
$R_{free}$ test set	4729 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtrriage
Anisotropy	0.171	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TN8, ZN, GOL, NAG

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	0.48	0/2309	0.78	0/3145
1	B	0.44	0/2311	0.75	2/3144 (0.1%)
All	All	0.46	0/4620	0.77	2/6289 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	ARG	CG-CD-NE	-5.62	99.99	111.80
1	B	136	ARG	CG-CD-NE	-5.40	100.46	111.80

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	2243	0	2169	19	0
1	B	2248	0	2190	19	0
2	A	23	0	0	0	0
2	B	23	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	28	0	26	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	28	0	26	9	0
5	A	6	0	8	0	0
6	A	248	0	0	5	0
6	B	218	0	0	6	0
All	All	5067	0	4419	40	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 4.

All (40) 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:189:ASN:HD21	4:B:404:NAG:C1	1.04	1.60
1:A:74:ASN:HD21	4:A:403:NAG:C1	1.02	1.59
1:B:74:ASN:HD21	4:B:403:NAG:C1	0.98	1.58
1:A:189:ASN:ND2	4:A:404:NAG:C1	1.70	1.51
1:B:74:ASN:ND2	4:B:403:NAG:C1	1.79	1.40
1:A:74:ASN:ND2	4:A:403:NAG:C1	1.87	1.38
1:B:189:ASN:ND2	4:B:404:NAG:C1	1.88	1.36
1:B:189:ASN:HD21	4:B:404:NAG:C2	1.92	0.80
1:B:298:ALA:CB	6:B:691:HOH:O	2.30	0.80
1:A:174:VAL:HG12	1:B:174:VAL:HG12	1.67	0.77
4:A:403:NAG:O4	6:A:501:HOH:O	2.02	0.76
1:A:74:ASN:HD21	4:A:403:NAG:C2	1.99	0.72
1:A:202:ASN:HA	6:A:619:HOH:O	1.90	0.71
1:B:298:ALA:HB2	6:B:691:HOH:O	1.90	0.71
1:A:74:ASN:ND2	4:A:403:NAG:C2	2.55	0.70
4:A:404:NAG:O4	6:A:502:HOH:O	2.09	0.70
1:B:189:ASN:ND2	4:B:404:NAG:C2	2.52	0.68
1:A:252:ARG:HB2	1:A:252:ARG:NH1	2.12	0.65
1:B:65:LYS:HE2	6:B:511:HOH:O	2.06	0.56
1:A:24:GLU:HB3	6:A:733:HOH:O	2.04	0.56
1:B:189:ASN:CG	4:B:404:NAG:C1	2.71	0.54
1:A:263:TYR:CD1	1:A:267:GLU:HG3	2.43	0.53
1:A:97:ASN:HB3	4:A:403:NAG:O7	2.10	0.52
1:A:252:ARG:HB2	1:A:252:ARG:CZ	2.40	0.52
1:B:74:ASN:ND2	4:B:403:NAG:C2	2.67	0.52
1:B:175:GLU:OE2	1:B:252:ARG:NH1	2.43	0.51
1:A:74:ASN:ND2	4:A:403:NAG:O5	2.34	0.50
1:A:189:ASN:CG	4:A:404:NAG:C1	2.69	0.49
1:B:189:ASN:ND2	4:B:404:NAG:O5	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ASN:HA	1:B:44:MET:HA	1.73	0.46
1:A:80:THR:OG1	1:A:205:THR:HG23	2.18	0.44
2:B:401:TN8:C2	2:B:401:TN8:SE	3.16	0.43
1:A:79:GLU:HG3	6:A:662:HOH:O	2.19	0.42
1:A:178:LYS:HE3	6:B:651:HOH:O	2.19	0.42
1:B:34:PRO:HA	1:B:37:TRP:CE2	2.55	0.42
1:A:26:SER:O	1:A:33:GLY:HA2	2.20	0.41
1:B:298:ALA:HB1	6:B:691:HOH:O	2.06	0.41
1:B:178:LYS:HD3	6:B:548:HOH:O	2.20	0.41
1:A:225:ARG:HD2	1:A:240:LEU:HD11	2.03	0.41
1:B:116:MET:HA	1:B:142:HIS:O	2.22	0.40

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	277/332 (83%)	264 (95%)	13 (5%)	0	100	100
1	B	276/332 (83%)	266 (96%)	10 (4%)	0	100	100
All	All	553/664 (83%)	530 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	250/297 (84%)	248 (99%)	2 (1%)	81	72
1	B	251/297 (84%)	248 (99%)	3 (1%)	71	57
All	All	501/594 (84%)	496 (99%)	5 (1%)	76	65

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ILE
1	A	263	TYR
1	B	158	ILE
1	B	193	VAL
1	B	263	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	197	GLN
1	B	74	ASN
1	B	189	ASN
1	B	202	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
4	NAG	B	403	-	14,14,15	1.12	0	17,19,21	1.57	4 (23%)
2	TN8	A	401	3	23,24,24	1.28	1 (4%)	31,33,33	0.54	0
4	NAG	A	403	-	14,14,15	0.86	0	17,19,21	1.75	4 (23%)
2	TN8	B	401	3	23,24,24	1.60	1 (4%)	31,33,33	0.84	1 (3%)
4	NAG	A	404	-	14,14,15	0.73	0	17,19,21	1.78	5 (29%)
5	GOL	A	405	-	5,5,5	0.27	0	5,5,5	0.76	0
4	NAG	B	404	-	14,14,15	0.81	0	17,19,21	1.48	3 (17%)

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
4	NAG	B	403	-	-	2/6/23/26	0/1/1/1
2	TN8	A	401	3	-	3/13/16/16	0/2/2/2
4	NAG	A	403	-	-	0/6/23/26	0/1/1/1
2	TN8	B	401	3	-	3/13/16/16	0/2/2/2
4	NAG	A	404	-	-	2/6/23/26	0/1/1/1
5	GOL	A	405	-	-	0/4/4/4	-
4	NAG	B	404	-	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	TN8	C-N2	7.23	1.39	1.30
2	A	401	TN8	C-N2	5.26	1.36	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	NAG	C1-O5-C5	-4.92	105.53	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	NAG	C1-O5-C5	3.97	117.57	112.19
2	B	401	TN8	C9-N2-C	3.72	129.06	121.60
4	B	404	NAG	C1-O5-C5	-3.50	107.44	112.19
4	A	404	NAG	C3-C4-C5	3.17	115.90	110.24
4	B	403	NAG	O7-C7-N2	3.07	127.59	121.95
4	A	403	NAG	C6-C5-C4	3.02	120.08	113.00
4	A	404	NAG	C8-C7-N2	3.02	121.21	116.10
4	B	403	NAG	C8-C7-N2	-2.67	111.58	116.10
4	B	403	NAG	O5-C5-C6	2.57	111.24	107.20
4	A	403	NAG	O5-C1-C2	-2.51	107.33	111.29
4	B	403	NAG	O4-C4-C5	2.38	115.22	109.30
4	A	404	NAG	O5-C5-C6	2.26	110.75	107.20
4	B	404	NAG	C6-C5-C4	2.22	118.21	113.00
4	B	404	NAG	O5-C1-C2	-2.14	107.91	111.29
4	A	404	NAG	O7-C7-C8	-2.03	118.29	122.06
4	A	403	NAG	O4-C4-C5	2.00	114.27	109.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

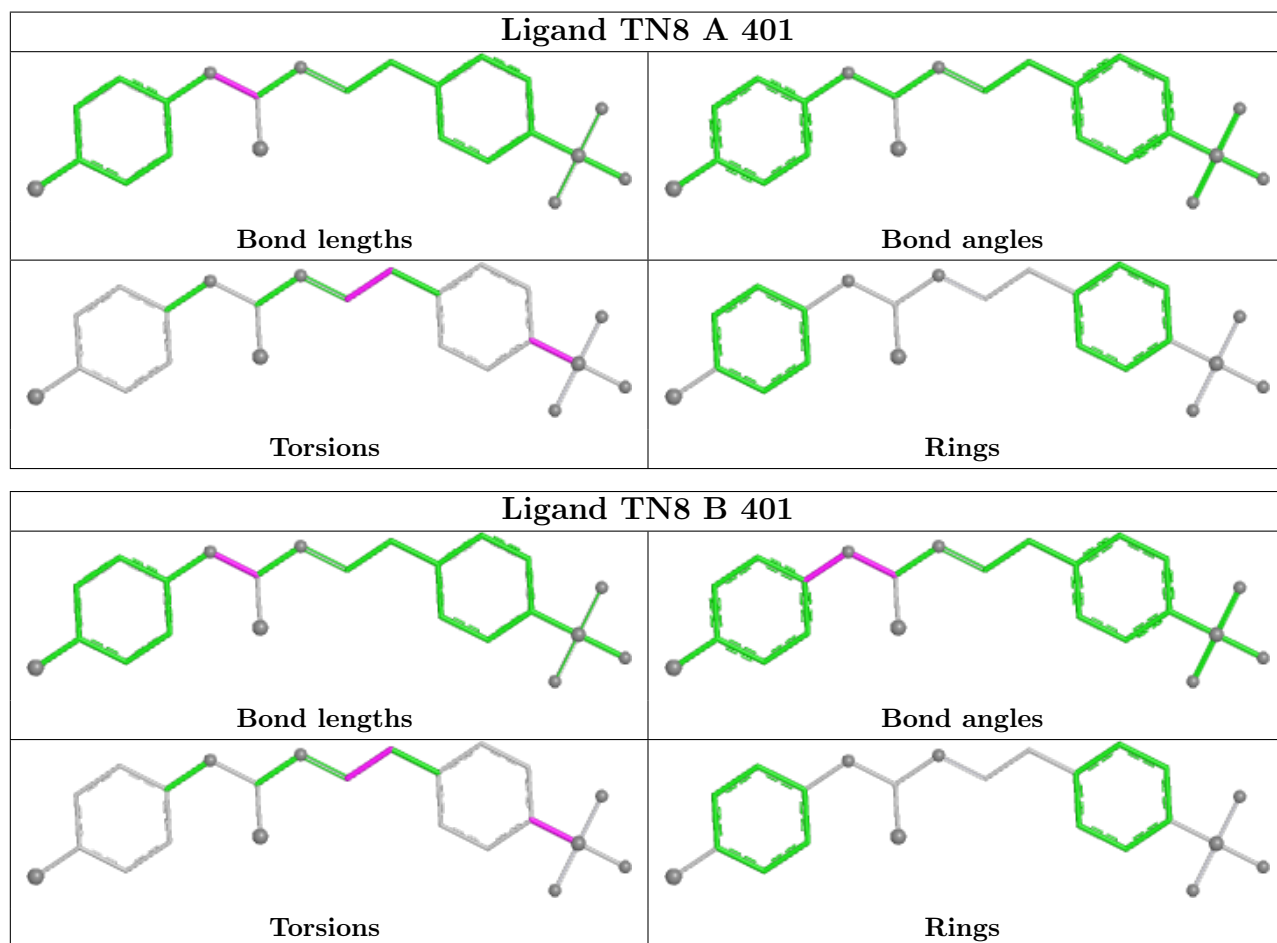
Mol	Chain	Res	Type	Atoms
4	A	404	NAG	C8-C7-N2-C2
4	A	404	NAG	O7-C7-N2-C2
4	B	403	NAG	C4-C5-C6-O6
4	B	403	NAG	O5-C5-C6-O6
2	A	401	TN8	N-C1-C2-C3
2	A	401	TN8	C7-C6-S-O
2	B	401	TN8	C7-C6-S-O
2	A	401	TN8	C5-C6-S-O
2	B	401	TN8	C5-C6-S-O
2	B	401	TN8	N-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	NAG	3	0
4	A	403	NAG	7	0
2	B	401	TN8	1	0
4	A	404	NAG	3	0
4	B	404	NAG	6	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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	277/332 (83%)	-0.11	8 (2%) 51 54	21, 28, 48, 73	0
1	B	277/332 (83%)	0.26	18 (6%) 18 19	20, 32, 55, 66	0
All	All	554/664 (83%)	0.07	26 (4%) 31 33	20, 30, 52, 73	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	GLN	3.8
1	A	31	LEU	3.8
1	A	30	ILE	3.5
1	B	264	GLY	3.4
1	B	78	THR	3.2
1	A	299	ARG	3.2
1	B	199	VAL	3.1
1	A	24	GLU	3.0
1	B	76	SER	2.9
1	B	198	PHE	2.7
1	B	265	SER	2.7
1	B	300	GLY	2.7
1	B	31	LEU	2.6
1	B	239	VAL	2.5
1	B	240	LEU	2.5
1	A	202	ASN	2.4
1	B	196	SER	2.4
1	B	271	ARG	2.4
1	B	167	LEU	2.4
1	B	201	PRO	2.3
1	B	75	THR	2.3
1	A	78	THR	2.1
1	A	201	PRO	2.1
1	B	270	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	300	GLY	2.1
1	B	164	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

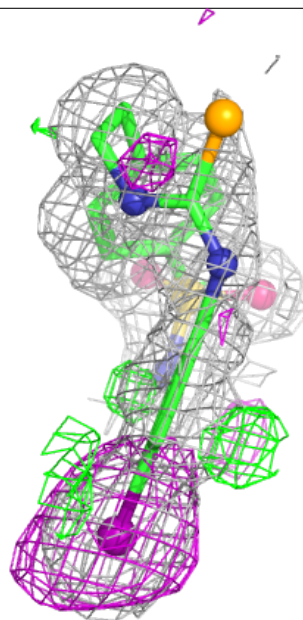
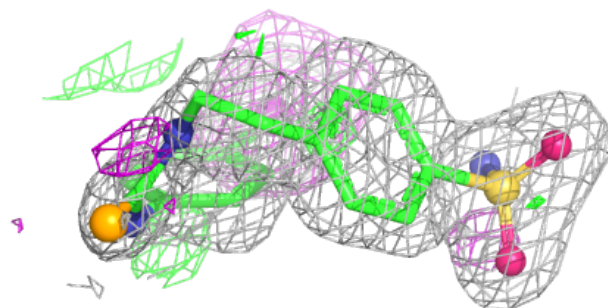
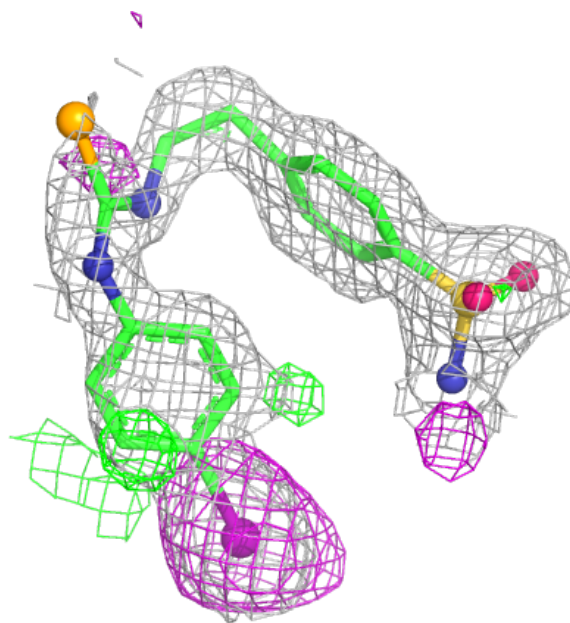
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

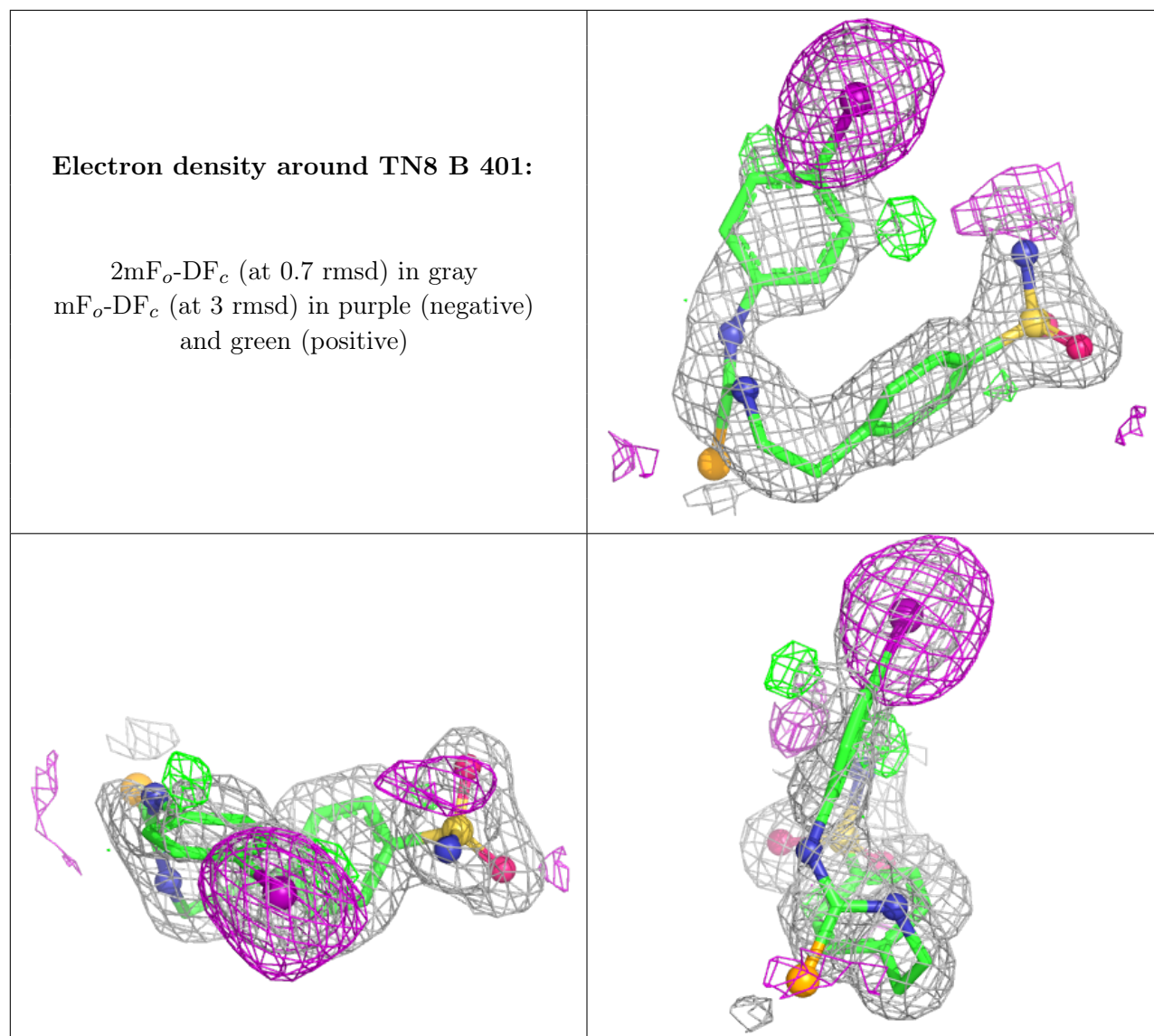
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	B	403	14/15	0.75	0.17	43,56,64,64	0
4	NAG	A	404	14/15	0.85	0.12	49,61,67,73	0
4	NAG	A	403	14/15	0.85	0.16	42,53,60,62	0
4	NAG	B	404	14/15	0.88	0.23	47,55,63,64	0
2	TN8	A	401	23/23	0.94	0.16	21,31,47,150	23
2	TN8	B	401	23/23	0.94	0.14	23,36,66,168	23
5	GOL	A	405	6/6	0.94	0.13	26,33,34,45	0
3	ZN	B	402	1/1	1.00	0.04	28,28,28,28	0
3	ZN	A	402	1/1	1.00	0.04	25,25,25,25	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 TN8 A 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.