



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:44 PM UTC

PDB ID : 7DVB / pdb\_00007dvb  
Title : D335N variant of Bt4394 in complex with 6SO3-NAG-oxazoline intermediate  
Authors : Zhang, Z.; He, Y.; Jin, Y.  
Deposited on : 2021-01-13  
Resolution : 2.05 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

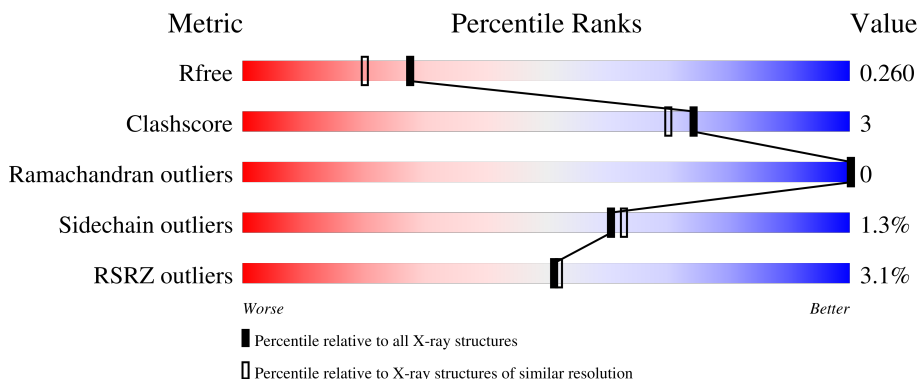
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	534	
1	B	534	
1	C	534	
1	D	534	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17255 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 Beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	507	4131	2658	704	753	16	0	1	0
1	B	508	4131	2658	704	753	16	0	0	0
1	C	519	4227	2716	721	774	16	0	1	0
1	D	518	4221	2713	721	771	16	0	1	0

There are 40 discrepancies between the modelled and reference sequences:

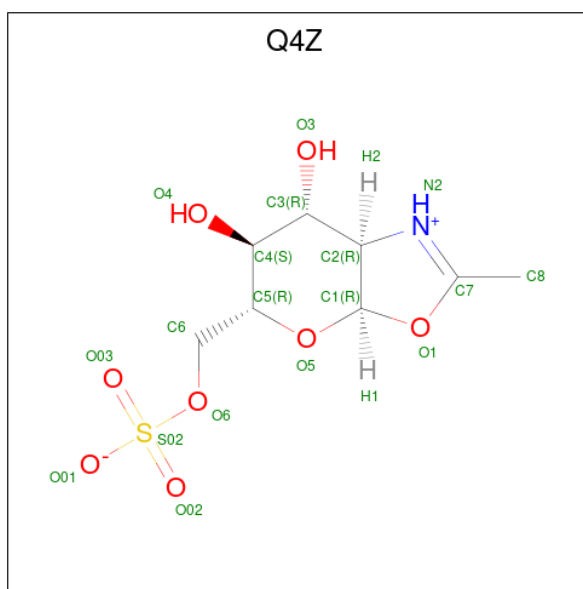
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	initiating methionine	UNP A0A0P0FIE8
A	335	ASN	ASP	engineered mutation	UNP A0A0P0FIE8
A	547	LEU	-	expression tag	UNP A0A0P0FIE8
A	548	GLU	-	expression tag	UNP A0A0P0FIE8
A	549	HIS	-	expression tag	UNP A0A0P0FIE8
A	550	HIS	-	expression tag	UNP A0A0P0FIE8
A	551	HIS	-	expression tag	UNP A0A0P0FIE8
A	552	HIS	-	expression tag	UNP A0A0P0FIE8
A	553	HIS	-	expression tag	UNP A0A0P0FIE8
A	554	HIS	-	expression tag	UNP A0A0P0FIE8
B	21	MET	-	initiating methionine	UNP A0A0P0FIE8
B	335	ASN	ASP	engineered mutation	UNP A0A0P0FIE8
B	547	LEU	-	expression tag	UNP A0A0P0FIE8
B	548	GLU	-	expression tag	UNP A0A0P0FIE8
B	549	HIS	-	expression tag	UNP A0A0P0FIE8
B	550	HIS	-	expression tag	UNP A0A0P0FIE8
B	551	HIS	-	expression tag	UNP A0A0P0FIE8
B	552	HIS	-	expression tag	UNP A0A0P0FIE8
B	553	HIS	-	expression tag	UNP A0A0P0FIE8
B	554	HIS	-	expression tag	UNP A0A0P0FIE8
C	21	MET	-	initiating methionine	UNP A0A0P0FIE8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	335	ASN	ASP	engineered mutation	UNP A0A0P0FIE8
C	547	LEU	-	expression tag	UNP A0A0P0FIE8
C	548	GLU	-	expression tag	UNP A0A0P0FIE8
C	549	HIS	-	expression tag	UNP A0A0P0FIE8
C	550	HIS	-	expression tag	UNP A0A0P0FIE8
C	551	HIS	-	expression tag	UNP A0A0P0FIE8
C	552	HIS	-	expression tag	UNP A0A0P0FIE8
C	553	HIS	-	expression tag	UNP A0A0P0FIE8
C	554	HIS	-	expression tag	UNP A0A0P0FIE8
D	21	MET	-	initiating methionine	UNP A0A0P0FIE8
D	335	ASN	ASP	engineered mutation	UNP A0A0P0FIE8
D	547	LEU	-	expression tag	UNP A0A0P0FIE8
D	548	GLU	-	expression tag	UNP A0A0P0FIE8
D	549	HIS	-	expression tag	UNP A0A0P0FIE8
D	550	HIS	-	expression tag	UNP A0A0P0FIE8
D	551	HIS	-	expression tag	UNP A0A0P0FIE8
D	552	HIS	-	expression tag	UNP A0A0P0FIE8
D	553	HIS	-	expression tag	UNP A0A0P0FIE8
D	554	HIS	-	expression tag	UNP A0A0P0FIE8

- Molecule 2 is [(3 {a} {R},5 {R},6 {S},7 {R},7 {a} {R})-2-methyl-6,7-bis(oxidanyl)-5,6,7,7 {a}-tetrahydro-3 {a} {H}-pyrano[3,2-d][1,3]oxazol-1-ium-5-yl]methyl sulfate (CCD ID: Q4Z) (formula: C<sub>8</sub>H<sub>13</sub>NO<sub>8</sub>S) (labeled as "Ligand of Interest" by depositor).



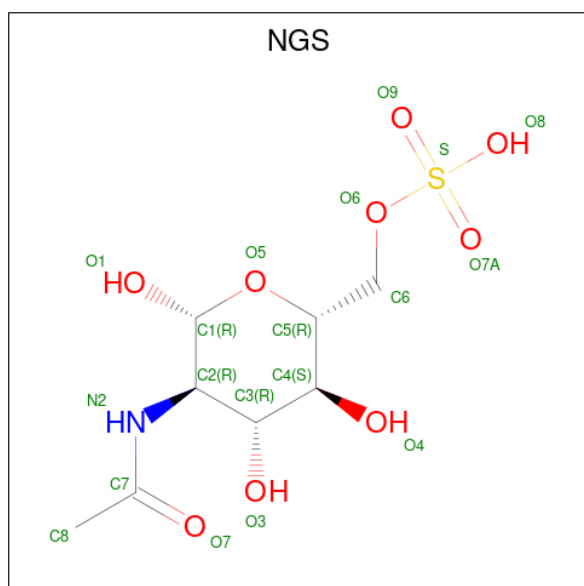
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			S
2	A	1	18	8	1	8	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			18	8	1	8	1		
2	C	1	Total	C	N	O	S	0	0
			18	8	1	8	1		
2	D	1	Total	C	N	O	S	0	0
			18	8	1	8	1		

- Molecule 3 is 2-acetamido-2-deoxy-6-O-sulfo-beta-D-glucopyranose (CCD ID: NGS) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>9</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	S	0	0
			19	8	1	9	1		

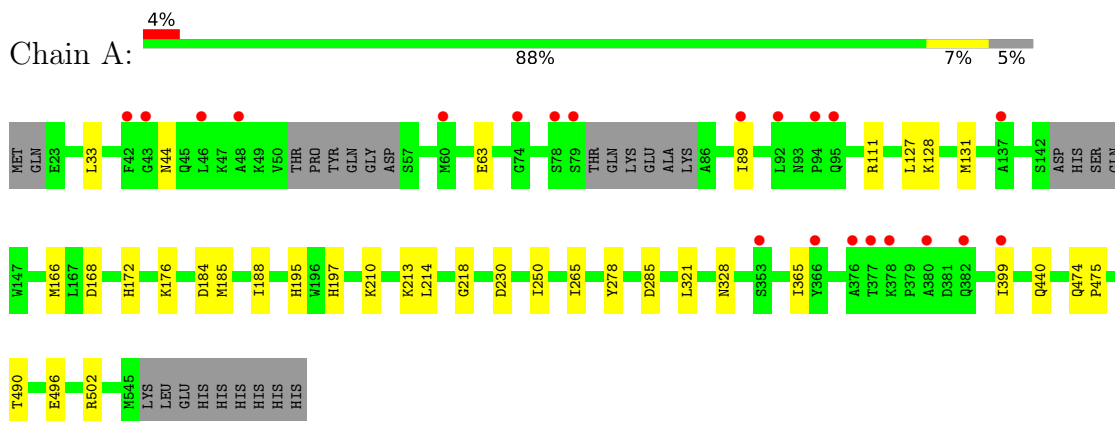
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total	O	0	0
			130	130		
4	B	125	Total	O	0	0
			125	125		
4	C	116	Total	O	0	0
			116	116		
4	D	83	Total	O	0	0
			83	83		

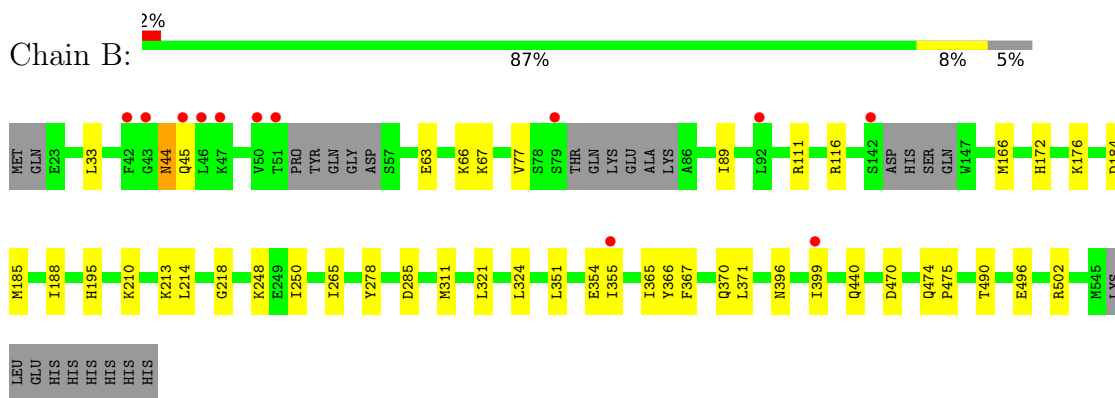
### 3 Residue-property plots [i](#)

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.

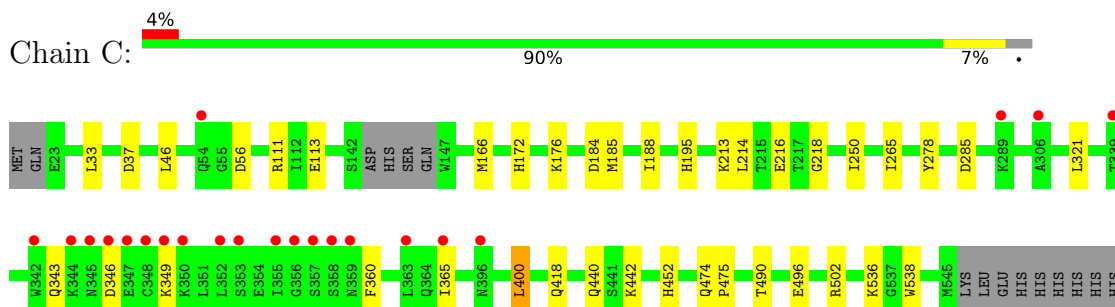
- Molecule 1: Beta-N-acetylhexosaminidase



- Molecule 1: Beta-N-acetylhexosaminidase



- Molecule 1: Beta-N-acetylhexosaminidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.03Å 67.00Å 192.80Å 90.00° 94.67° 90.00°	Depositor
Resolution (Å)	19.72 – 2.05 19.72 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.72-2.05) 99.2 (19.72-2.05)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.06Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.229 , 0.259 0.229 , 0.260	Depositor DCC
$R_{free}$ test set	6601 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtrriage
Anisotropy	0.215	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 30.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17255	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0940e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: NGS, Q4Z

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	0.45	0/4235	0.88	0/5727
1	B	0.45	0/4235	0.88	0/5727
1	C	0.45	0/4335	0.88	0/5865
1	D	0.46	0/4329	0.89	2/5857 (0.0%)
All	All	0.45	0/17134	0.88	2/23176 (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	D	328	ASN	CA-CB-CG	6.65	119.25	112.60
1	D	63	GLU	CB-CG-CD	5.96	122.72	112.60

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	4131	0	4098	21	0
1	B	4131	0	4099	31	0
1	C	4227	0	4189	25	0
1	D	4221	0	4186	33	0
2	A	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	18	0	0	0	0
2	C	18	0	0	0	0
2	D	18	0	0	0	0
3	D	19	0	9	1	0
4	A	130	0	0	0	0
4	B	125	0	0	0	0
4	C	116	0	0	0	0
4	D	83	0	0	1	0
All	All	17255	0	16581	104	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 3.

All (104) 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:C:111:ARG:NH1	1:C:113:GLU:OE2	2.23	0.71
1:A:127:LEU:HD23	1:A:131:MET:HE2	1.77	0.67
1:C:265:ILE:CG1	1:C:321:LEU:HD11	2.27	0.64
1:D:265:ILE:CG1	1:D:321:LEU:HD11	2.26	0.64
1:B:367:PHE:HA	1:B:370:GLN:OE1	1.97	0.64
1:D:265:ILE:HG12	1:D:321:LEU:HD11	1.80	0.63
1:B:265:ILE:CG1	1:B:321:LEU:HD11	2.28	0.63
1:A:265:ILE:CG1	1:A:321:LEU:HD11	2.28	0.63
1:D:89:ILE:HD12	1:D:111:ARG:HH22	1.63	0.63
1:C:265:ILE:HG12	1:C:321:LEU:HD11	1.82	0.62
1:C:365:ILE:HG22	1:C:400:LEU:HD13	1.83	0.61
1:B:89:ILE:CG2	1:B:111:ARG:HG2	2.32	0.59
1:B:396:ASN:O	1:B:399:ILE:HG22	2.03	0.59
1:B:265:ILE:HG12	1:B:321:LEU:HD11	1.85	0.58
1:A:265:ILE:HG12	1:A:321:LEU:HD11	1.85	0.58
1:A:127:LEU:CD2	1:A:131:MET:HE2	2.35	0.55
1:B:44:ASN:HB3	1:D:248:LYS:HD3	1.89	0.54
1:B:45:GLN:HB3	1:D:323:GLU:HG2	1.88	0.54
1:D:46:LEU:HD11	1:D:87:ARG:HH11	1.72	0.54
1:C:185:MET:HE1	1:C:496:GLU:HG2	1.89	0.54
1:D:185:MET:HE1	1:D:496:GLU:HG2	1.89	0.54
1:A:185:MET:HE1	1:A:496:GLU:HG2	1.90	0.54
1:B:185:MET:HE1	1:B:496:GLU:HG2	1.89	0.53
1:B:311:MET:HE1	1:B:371:LEU:HG	1.90	0.53
1:D:109:GLN:HE22	1:D:111:ARG:NH2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:LYS:HG3	1:D:250:ILE:HD11	1.91	0.52
1:C:418:GLN:NE2	1:C:418:GLN:HA	2.24	0.51
1:D:346:ASP:HA	1:D:349:LYS:HE3	1.93	0.50
1:A:176:LYS:HG3	1:A:250:ILE:HD11	1.93	0.50
1:C:176:LYS:HG3	1:C:250:ILE:HD11	1.93	0.50
1:C:265:ILE:HG13	1:C:321:LEU:HD11	1.93	0.50
1:C:213:LYS:HA	1:C:216:GLU:HB2	1.94	0.49
1:B:265:ILE:HG13	1:B:321:LEU:HD11	1.94	0.49
1:D:297:GLY:HA2	3:D:602:NGS:O3	2.12	0.49
1:B:176:LYS:HG3	1:B:250:ILE:HD11	1.94	0.49
1:A:128:LYS:HA	1:A:131:MET:HE3	1.95	0.49
1:D:265:ILE:HG13	1:D:321:LEU:HD11	1.94	0.48
1:D:536:LYS:HE2	1:D:538:TRP:CZ2	2.49	0.48
1:A:265:ILE:HG13	1:A:321:LEU:HD11	1.94	0.47
1:D:29:GLN:OE1	1:D:30:PRO:HD2	2.14	0.47
1:B:351:LEU:HA	1:B:354:GLU:HG2	1.97	0.47
1:C:365:ILE:CG2	1:C:400:LEU:HD13	2.45	0.47
1:D:46:LEU:HD11	1:D:87:ARG:HD3	1.97	0.46
1:C:346:ASP:HA	1:C:349:LYS:HE3	1.97	0.46
1:B:365:ILE:HG22	1:B:399:ILE:CG2	2.45	0.46
1:B:470:ASP:HA	1:C:452:HIS:HD2	1.80	0.46
1:D:184:ASP:O	1:D:188:ILE:HG12	2.16	0.46
1:A:285:ASP:OD1	1:A:285:ASP:N	2.49	0.45
1:D:89:ILE:HD12	1:D:111:ARG:NH2	2.31	0.45
1:A:172:HIS:CE1	1:A:490[B]:THR:HG22	2.51	0.45
1:D:289:LYS:HD2	1:D:291:GLU:OE2	2.16	0.45
1:B:285:ASP:OD1	1:B:285:ASP:N	2.49	0.45
1:B:172:HIS:CE1	1:B:490:THR:HG22	2.52	0.45
1:D:172:HIS:CE1	1:D:490:THR:HG22	2.51	0.45
1:C:172:HIS:CE1	1:C:490:THR:HG22	2.52	0.45
1:C:184:ASP:O	1:C:188:ILE:HG12	2.17	0.45
1:C:285:ASP:N	1:C:285:ASP:OD1	2.48	0.44
1:A:184:ASP:O	1:A:188:ILE:HG12	2.17	0.44
1:D:109:GLN:HE22	1:D:111:ARG:HH21	1.65	0.44
1:B:470:ASP:HA	1:C:452:HIS:CD2	2.52	0.44
1:D:109:GLN:NE2	1:D:111:ARG:HH21	2.14	0.44
1:B:366:TYR:HD1	1:B:399:ILE:HD11	1.83	0.44
1:B:45:GLN:CB	1:D:323:GLU:HG2	2.48	0.43
1:C:214:LEU:O	1:C:218:GLY:HA3	2.18	0.43
1:D:166:MET:HG3	1:D:195:HIS:CG	2.54	0.43
1:D:53:TYR:CD2	1:D:57:SER:OG	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:MET:HG3	1:B:195:HIS:CG	2.54	0.43
1:C:343:GLN:HA	1:C:360:PHE:CE1	2.53	0.43
1:C:440:GLN:HB3	1:C:502:ARG:CZ	2.49	0.43
1:B:184:ASP:O	1:B:188:ILE:HG12	2.17	0.43
1:A:89:ILE:HG23	1:A:111:ARG:HG3	2.01	0.43
1:B:214:LEU:O	1:B:218:GLY:HA3	2.19	0.43
1:C:166:MET:HG3	1:C:195:HIS:CG	2.54	0.43
1:B:311:MET:CE	1:B:371:LEU:CD2	2.96	0.43
1:D:440:GLN:HB3	1:D:502:ARG:CZ	2.49	0.42
1:A:166:MET:HG3	1:A:195:HIS:CG	2.53	0.42
1:B:474:GLN:N	1:B:475:PRO:CD	2.82	0.42
1:D:285:ASP:N	1:D:285:ASP:OD1	2.49	0.42
1:A:365:ILE:HG22	1:A:399:ILE:CG1	2.50	0.42
1:B:355:ILE:HG22	1:B:355:ILE:O	2.19	0.42
1:D:213:LYS:HB2	1:D:278:TYR:CZ	2.54	0.42
1:D:474:GLN:N	1:D:475:PRO:CD	2.82	0.42
1:A:440:GLN:HB3	1:A:502:ARG:CZ	2.49	0.42
1:C:474:GLN:N	1:C:475:PRO:CD	2.83	0.42
1:D:214:LEU:O	1:D:218:GLY:HA3	2.19	0.42
1:A:213:LYS:HB2	1:A:278:TYR:CZ	2.54	0.42
1:B:66:LYS:HE3	1:B:77:VAL:O	2.20	0.42
1:D:520:GLU:HG2	4:D:774:HOH:O	2.19	0.42
1:A:214:LEU:O	1:A:218:GLY:HA3	2.20	0.42
1:B:213:LYS:HB2	1:B:278:TYR:CZ	2.55	0.42
1:B:248:LYS:HE3	1:B:324:LEU:HD23	2.01	0.42
1:B:440:GLN:HB3	1:B:502:ARG:CZ	2.50	0.42
1:C:213:LYS:HB2	1:C:278:TYR:CZ	2.54	0.42
1:D:46:LEU:CD1	1:D:87:ARG:HH11	2.32	0.41
1:A:474:GLN:N	1:A:475:PRO:CD	2.83	0.41
1:D:166:MET:HA	1:D:195:HIS:O	2.21	0.41
1:A:230:ASP:OD2	1:C:442:LYS:HE3	2.21	0.41
1:C:166:MET:HA	1:C:195:HIS:O	2.21	0.41
1:B:365:ILE:HG22	1:B:399:ILE:HG23	2.01	0.41
1:B:166:MET:HA	1:B:195:HIS:O	2.20	0.41
1:C:536:LYS:HE2	1:C:538:TRP:CZ2	2.56	0.41
1:D:222:ASN:ND2	1:D:237:ARG:HD3	2.36	0.41
1:A:166:MET:HA	1:A:195:HIS:O	2.21	0.40
1:A:168:ASP:HA	1:A:197:HIS:HB3	2.04	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	500/534 (94%)	494 (99%)	6 (1%)	0	100	100
1	B	500/534 (94%)	494 (99%)	6 (1%)	0	100	100
1	C	516/534 (97%)	508 (98%)	8 (2%)	0	100	100
1	D	515/534 (96%)	507 (98%)	8 (2%)	0	100	100
All	All	2031/2136 (95%)	2003 (99%)	28 (1%)	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	435/459 (95%)	430 (99%)	5 (1%)	65	68
1	B	435/459 (95%)	429 (99%)	6 (1%)	59	60
1	C	445/459 (97%)	440 (99%)	5 (1%)	65	68
1	D	444/459 (97%)	438 (99%)	6 (1%)	59	60
All	All	1759/1836 (96%)	1737 (99%)	22 (1%)	61	63

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	44	ASN

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Mol	Chain	Res	Type
1	A	63	GLU
1	A	210	LYS
1	A	328	ASN
1	B	33	LEU
1	B	44	ASN
1	B	63	GLU
1	B	67	LYS
1	B	116	ARG
1	B	210	LYS
1	C	33	LEU
1	C	37	ASP
1	C	46	LEU
1	C	56	ASP
1	C	400	LEU
1	D	33	LEU
1	D	44	ASN
1	D	56	ASP
1	D	63	GLU
1	D	76	LYS
1	D	328	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	ASN
1	A	343	GLN
1	A	440	GLN
1	B	222	ASN
1	B	343	GLN
1	C	45	GLN
1	C	70	GLN
1	C	222	ASN
1	C	418	GLN
1	C	422	GLN
1	C	452	HIS
1	D	44	ASN
1	D	109	GLN
1	D	222	ASN
1	D	328	ASN
1	D	382	GLN
1	D	385	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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	Q4Z	B	601	-	18,19,19	0.55	0	21,29,29	1.31	2 (9%)
2	Q4Z	D	601	-	18,19,19	0.59	0	21,29,29	1.55	2 (9%)
2	Q4Z	C	601	-	18,19,19	0.66	1 (5%)	21,29,29	1.59	3 (14%)
3	NGS	D	602	-	19,19,19	0.40	0	27,28,28	0.72	0
2	Q4Z	A	601	-	18,19,19	0.51	0	21,29,29	1.56	2 (9%)

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	Q4Z	B	601	-	-	0/6/34/34	0/2/2/2
2	Q4Z	D	601	-	-	0/6/34/34	0/2/2/2
2	Q4Z	C	601	-	-	1/6/34/34	0/2/2/2
3	NGS	D	602	-	-	0/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Q4Z	A	601	-	-	1/6/34/34	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	Q4Z	O6-S02	2.06	1.62	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	Q4Z	C2-N2-C7	5.49	110.27	106.43
2	A	601	Q4Z	C2-N2-C7	5.42	110.22	106.43
2	D	601	Q4Z	C2-N2-C7	5.08	109.99	106.43
2	B	601	Q4Z	C2-N2-C7	4.08	109.28	106.43
2	D	601	Q4Z	C1-O5-C5	3.24	120.05	113.72
2	C	601	Q4Z	C1-O5-C5	2.97	119.51	113.72
2	A	601	Q4Z	C1-O5-C5	2.79	119.18	113.72
2	B	601	Q4Z	C1-O5-C5	2.77	119.13	113.72
2	C	601	Q4Z	O6-C6-C5	2.16	111.42	107.57

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	Q4Z	O5-C5-C6-O6
2	C	601	Q4Z	O5-C5-C6-O6

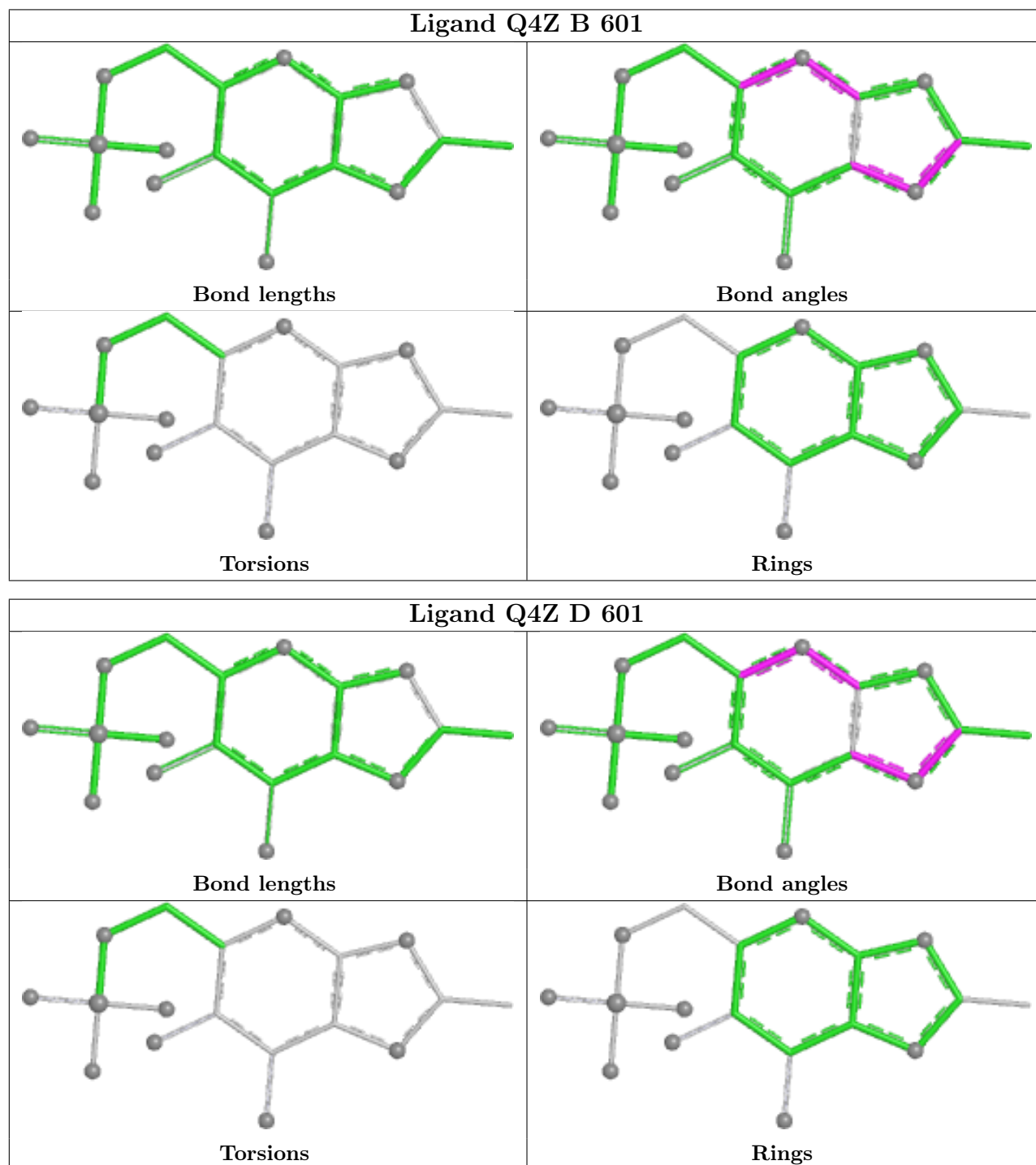
There are no ring outliers.

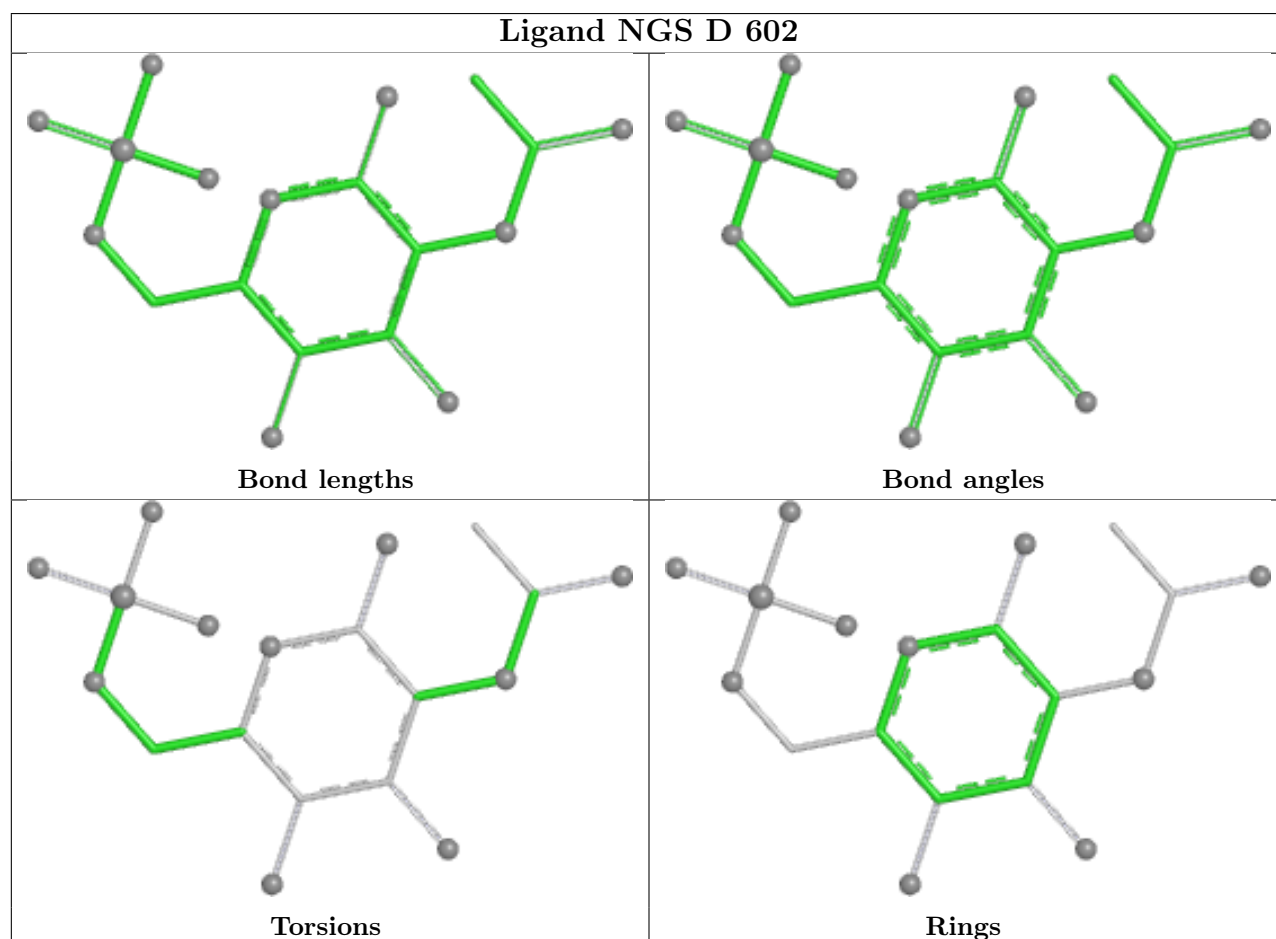
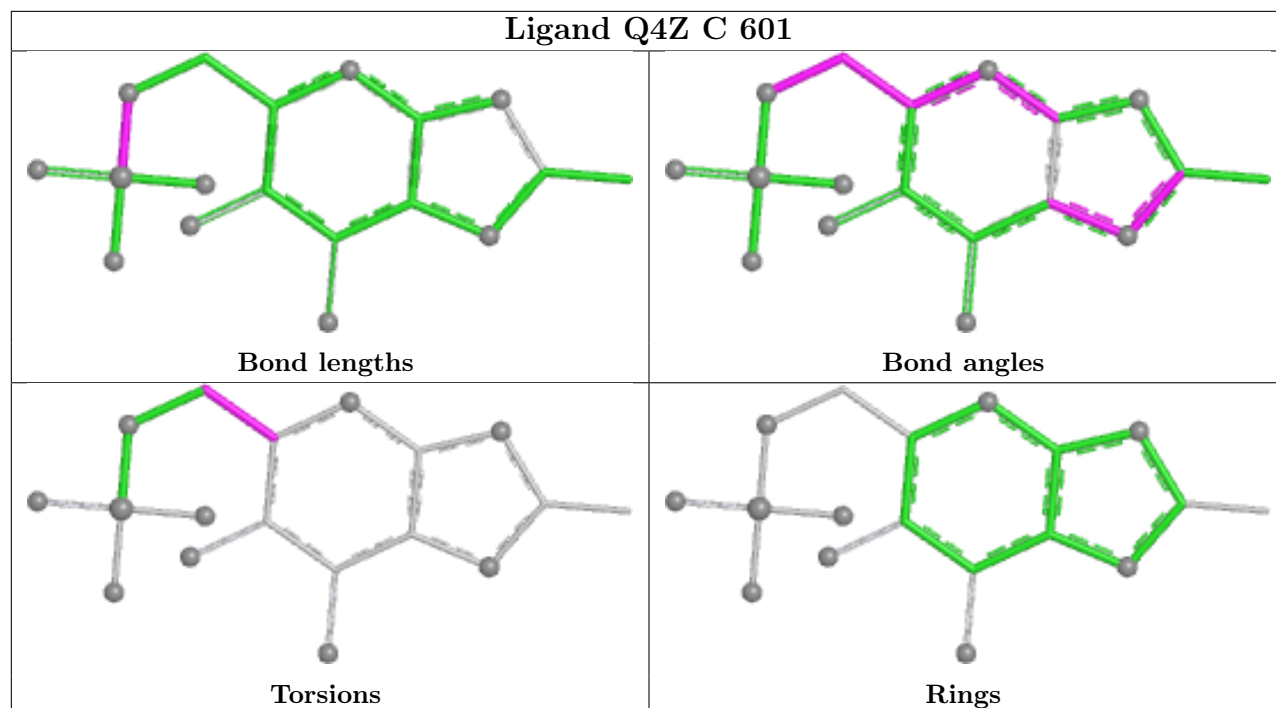
1 monomer is involved in 1 short contact:

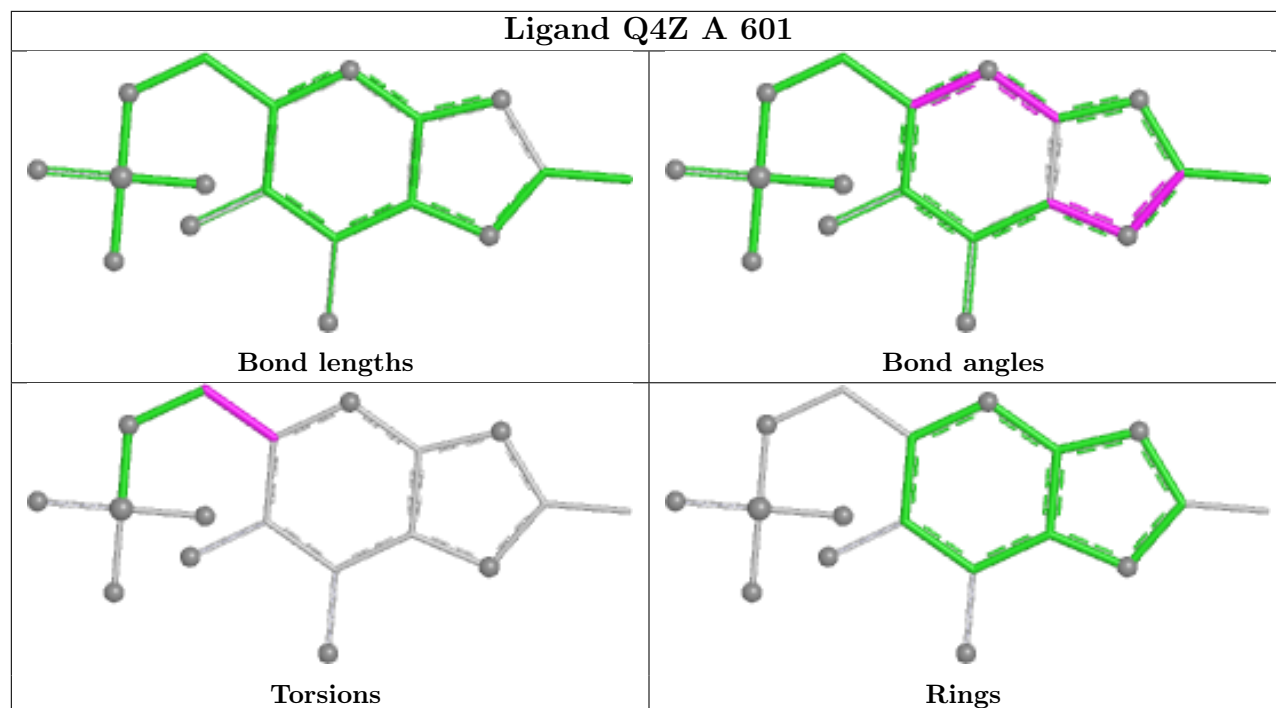
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	NGS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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, 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	507/534 (94%)	0.13	21 (4%) 41 41	14, 33, 57, 71	34 (6%)
1	B	508/534 (95%)	0.06	12 (2%) 59 61	20, 34, 56, 71	25 (4%)
1	C	519/534 (97%)	0.20	22 (4%) 40 40	18, 36, 57, 91	31 (5%)
1	D	518/534 (97%)	0.19	9 (1%) 69 70	19, 36, 56, 67	29 (5%)
All	All	2052/2136 (96%)	0.15	64 (3%) 51 52	14, 35, 57, 91	119 (5%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	353	SER	4.8
1	C	355	ILE	4.3
1	D	44	ASN	4.2
1	C	358	SER	4.2
1	D	43	GLY	3.8
1	B	43	GLY	3.6
1	C	349	LYS	3.6
1	C	54	GLN	3.6
1	A	89	ILE	3.6
1	A	79	SER	3.5
1	C	396	ASN	3.2
1	B	355	ILE	3.1
1	C	356	GLY	3.1
1	B	46	LEU	3.1
1	A	92	LEU	3.1
1	A	378	LYS	3.1
1	A	43	GLY	3.0
1	A	46	LEU	3.0
1	D	46	LEU	3.0
1	C	346	ASP	2.9
1	C	345	ASN	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	60	MET	2.8
1	B	45	GLN	2.8
1	C	357	SER	2.8
1	D	56	ASP	2.8
1	A	74	GLY	2.8
1	A	94	PRO	2.8
1	C	348	CYS	2.8
1	A	380	ALA	2.6
1	A	399	ILE	2.6
1	C	363	LEU	2.6
1	C	359	ASN	2.5
1	A	95	GLN	2.5
1	D	54	GLN	2.5
1	B	47	LYS	2.5
1	D	82	LYS	2.5
1	B	79	SER	2.5
1	B	399	ILE	2.5
1	A	48	ALA	2.4
1	A	353	SER	2.4
1	A	366	TYR	2.4
1	D	358	SER	2.4
1	A	78	SER	2.4
1	B	51	THR	2.4
1	C	350	LYS	2.4
1	C	344	LYS	2.3
1	D	399	ILE	2.3
1	B	92	LEU	2.3
1	C	352	LEU	2.3
1	B	50	VAL	2.2
1	A	382	GLN	2.2
1	C	289	LYS	2.2
1	A	376	ALA	2.1
1	C	306	ALA	2.1
1	A	377	THR	2.1
1	D	287	ARG	2.1
1	B	142	SER	2.1
1	B	42	PHE	2.1
1	A	137	ALA	2.1
1	C	365	ILE	2.1
1	A	42	PHE	2.1
1	C	347	GLU	2.0
1	C	342	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	339	THR	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](#)

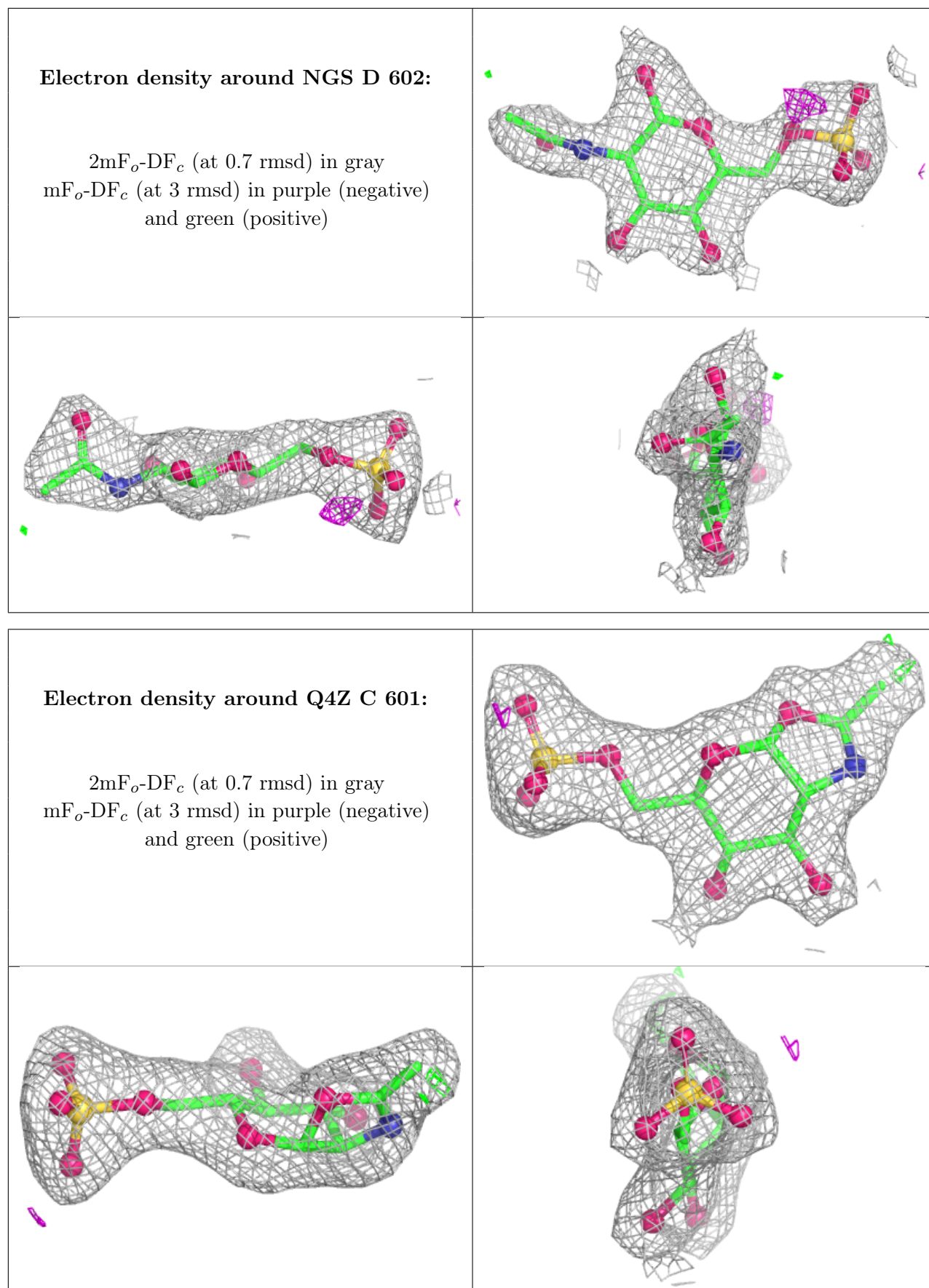
There are no oligosaccharides in this entry.

## 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, 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.

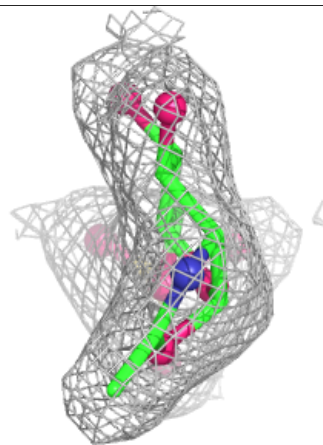
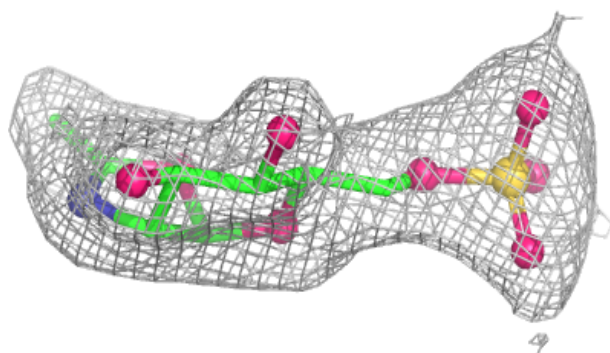
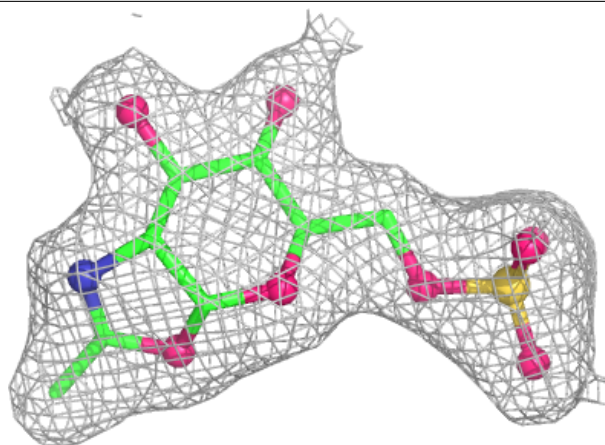
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NGS	D	602	19/19	0.84	0.12	49,55,64,65	0
2	Q4Z	C	601	18/18	0.97	0.06	26,27,28,29	0
2	Q4Z	B	601	18/18	0.97	0.05	24,27,30,30	0
2	Q4Z	D	601	18/18	0.98	0.05	26,27,28,29	0
2	Q4Z	A	601	18/18	0.98	0.05	21,22,27,28	0

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.



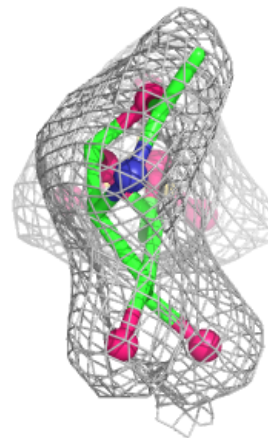
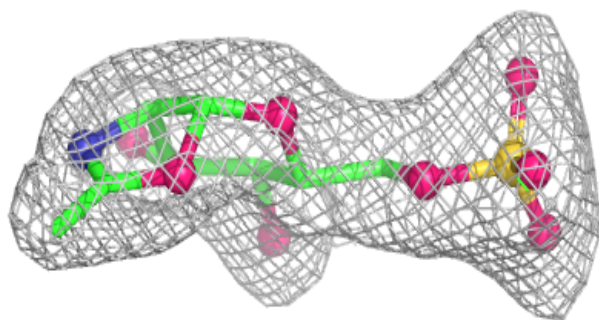
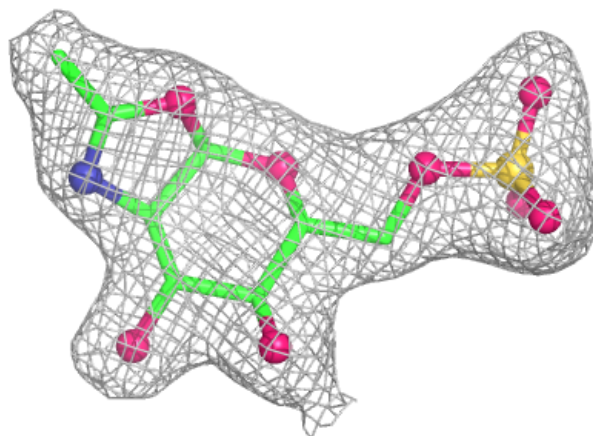
**Electron density around Q4Z B 601:**

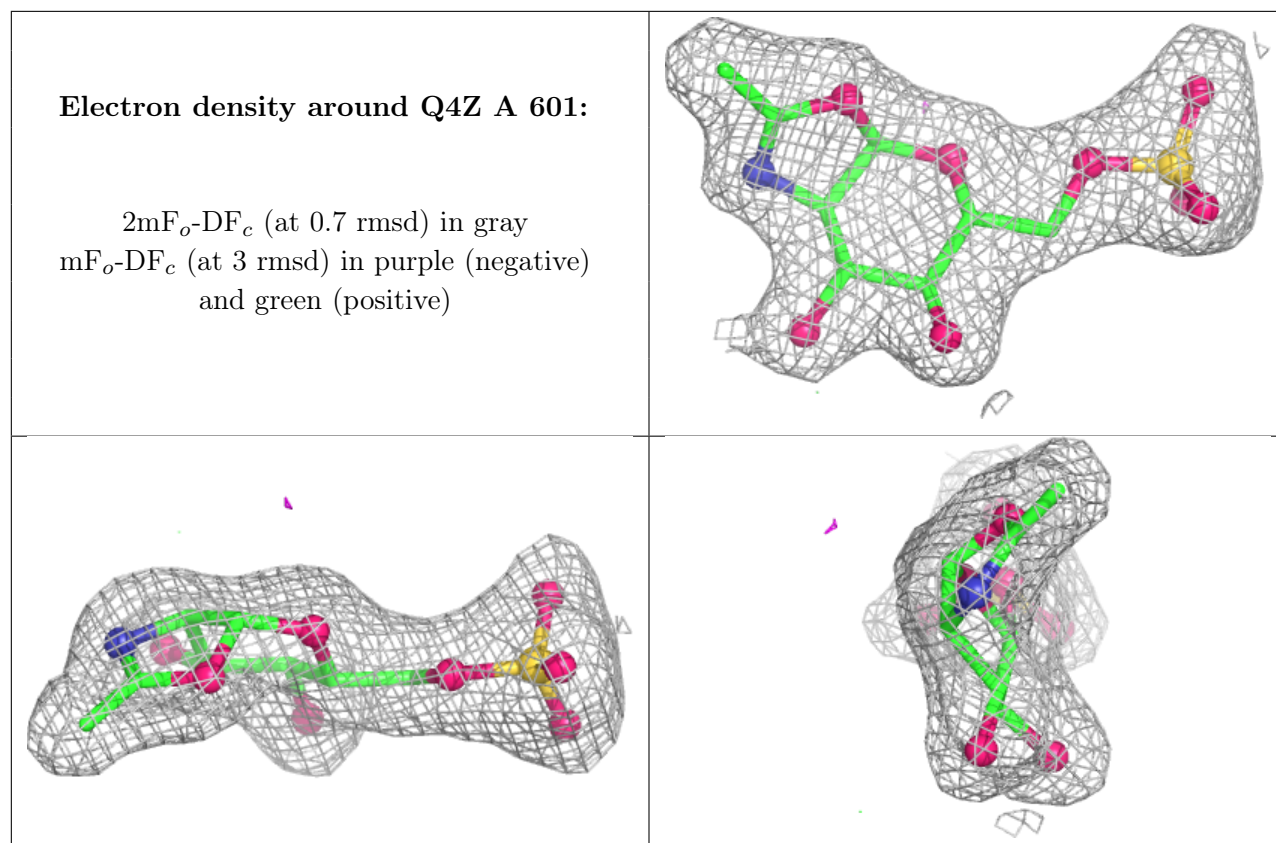
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Q4Z D 601:**

$2mF_o-DF_c$  (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.