



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 12:28 am GMT

PDB ID : 6S24  
Title : Crystal structure of the TgGalNAc-T3 in complex with UDP, manganese and the peptide 3  
Authors : de las Rivas, M.; Daniel, E.J.P.; Narimatsu, Y.; Companon, I.; Kato, K.; Hermosilla, P.; Thureau, A.; Ceballos-Laita, L.; Coelho, H.; Bernado, P.; Marcelo, F.; Hansen, L.; Lostao, A.; Corzana, F.; Clausen, H.; Gerken, T.A.; Hurtado-Guerrero, R.  
Deposited on : 2019-06-20  
Resolution : 2.12 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>.

---

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 : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)

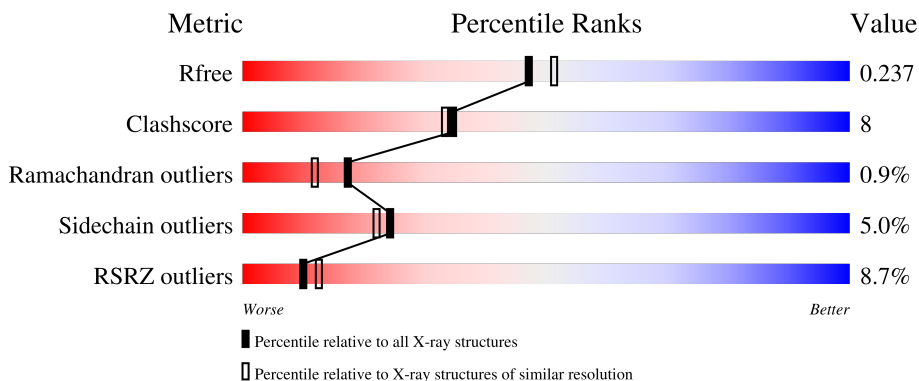
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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  $\geq 3$ , 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	631	
2	F	14	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

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
3	TAM	A	701	-	-	X	-
4	PO4	A	704	-	-	-	X
4	PO4	A	715	-	-	-	X
8	NGA	F	101	X	-	-	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4756 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.

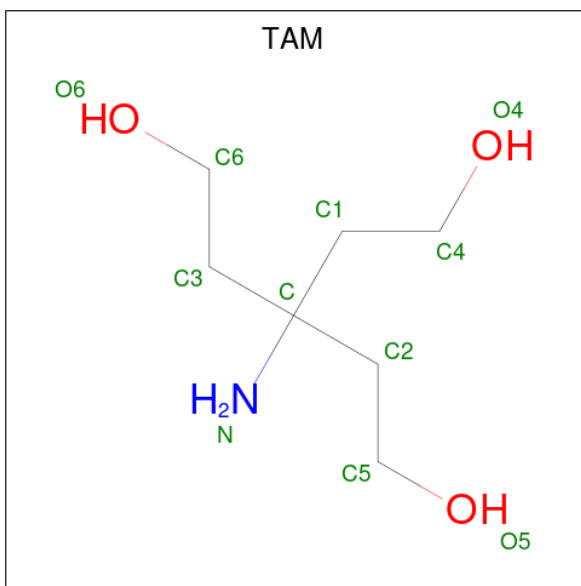
- Molecule 1 is a protein called Polypeptide N-acetylgalactosaminyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	537	4335	2760	753	799	23	0	0	0

- Molecule 2 is a protein called ALA-THR-GLY-ALA-GLY-ALA-GLY-ALA-GLY-THR-THR-PRO-GLY-PRO.

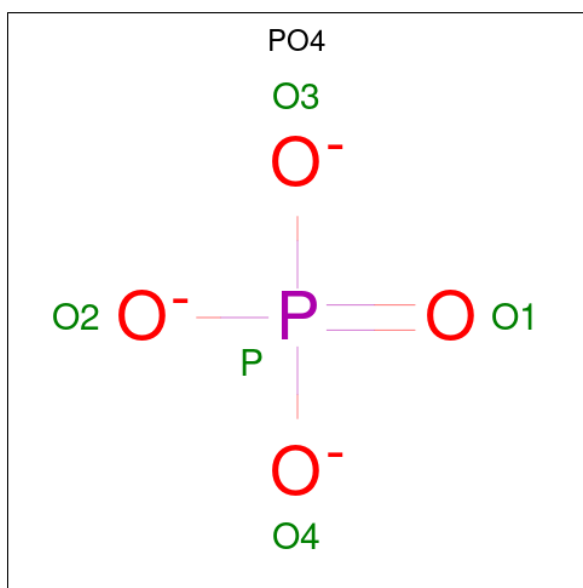
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	F	14	75	44	14	17	0	0	0

- Molecule 3 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: C<sub>7</sub>H<sub>17</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	11	7	1	3	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



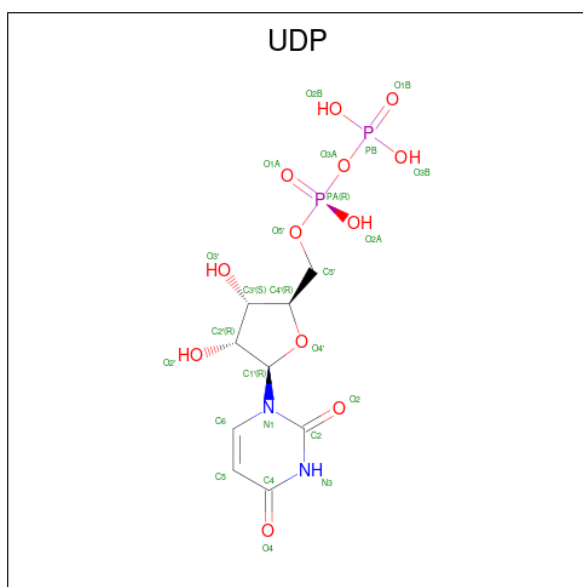
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

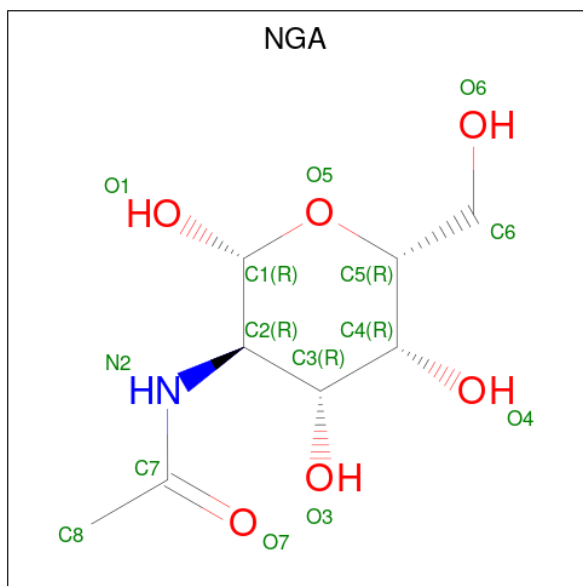
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mn	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-galactopyranose (three-letter code: NGA) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is water.

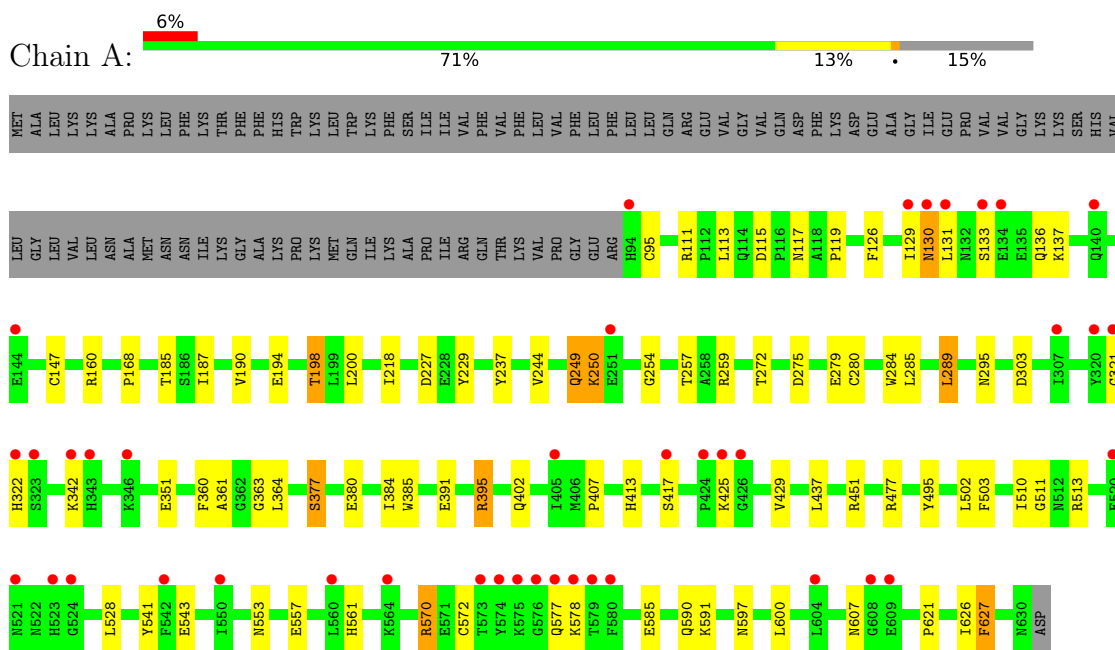
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
9	A	200	Total 200	O 200	0	0
9	F	1	Total 1	O 1	0	0



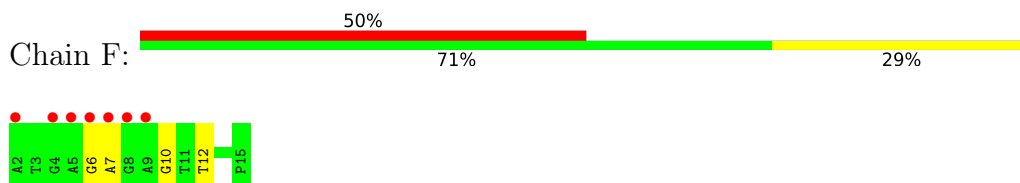
### 3 Residue-property plots

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: Polypeptide N-acetylgalactosaminyltransferase



- Molecule 2: ALA-THR-GLY-ALA-GLY-ALA-GLY-ALA-GLY-THR-THR-PRO-GLY-PRO



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.66Å 104.66Å 143.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.12 19.96 – 2.12	Depositor EDS
% Data completeness (in resolution range)	93.8 (19.96-2.12) 93.9 (19.96-2.12)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.13Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.191 , 0.237 0.199 , 0.237	Depositor DCC
$R_{free}$ test set	1655 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtrriage
Anisotropy	0.279	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4756	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: NGA, PO4, NAG, MN, TAM, UDP

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	0.71	0/4456	0.89	5/6037 (0.1%)
2	F	0.83	0/76	0.93	0/104
All	All	0.72	0/4532	0.89	5/6141 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	111	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	A	395	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	111	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	591	LYS	CB-CA-C	-5.01	100.38	110.40

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	4335	0	4198	62	0
2	F	75	0	68	7	0
3	A	11	0	17	30	0
4	A	75	0	0	1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	5	0	0	0	0
5	A	25	0	11	4	0
6	A	1	0	0	0	0
7	A	14	0	13	0	0
8	F	14	0	13	0	0
9	A	200	0	0	2	0
9	F	1	0	0	0	0
All	All	4756	0	4320	74	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 8.

All (74) 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)
3:A:701:TAM:H22	5:A:717:UDP:O3B	1.69	0.92
1:A:364:LEU:HD13	3:A:701:TAM:H12	1.56	0.87
1:A:361:ALA:HB3	3:A:701:TAM:H61	1.58	0.85
1:A:147:CYS:SG	9:A:985:HOH:O	2.35	0.84
1:A:275:ASP:OD2	3:A:701:TAM:H21	1.77	0.83
1:A:361:ALA:CB	3:A:701:TAM:H61	2.08	0.83
3:A:701:TAM:H62	3:A:701:TAM:O4	1.81	0.81
1:A:570:ARG:NH2	4:A:706:PO4:O3	2.22	0.73
1:A:477:ARG:HD3	9:A:952:HOH:O	1.90	0.71
3:A:701:TAM:O4	3:A:701:TAM:N	2.24	0.69
1:A:160:ARG:HD3	1:A:279:GLU:OE1	1.93	0.67
1:A:363:GLY:HA3	3:A:701:TAM:H31	1.75	0.67
1:A:200:LEU:HD23	1:A:237:TYR:CE2	2.29	0.66
3:A:701:TAM:C2	5:A:717:UDP:O3B	2.42	0.66
1:A:200:LEU:CD2	1:A:237:TYR:CE2	2.80	0.64
1:A:249:GLN:OE1	1:A:257:THR:HG22	1.98	0.64
1:A:259:ARG:NH2	1:A:363:GLY:HA2	2.12	0.64
1:A:597:ASN:HD22	1:A:600:LEU:H	1.46	0.63
1:A:259:ARG:HH22	1:A:363:GLY:HA2	1.63	0.62
1:A:503:PHE:CE1	1:A:627:PHE:CD1	2.89	0.61
1:A:119:PRO:HB3	1:A:126:PHE:CE1	2.37	0.59
1:A:131:LEU:O	1:A:136:GLN:NE2	2.32	0.59
1:A:363:GLY:CA	3:A:701:TAM:H31	2.33	0.58
1:A:194:GLU:OE2	1:A:198:THR:CG2	2.51	0.58
3:A:701:TAM:HN2	2:F:12:THR:CB	2.18	0.57
1:A:363:GLY:N	3:A:701:TAM:H31	2.20	0.56

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LEU:N	3:A:701:TAM:O6	2.38	0.56
1:A:377:SER:O	1:A:395:ARG:NH2	2.38	0.56
1:A:363:GLY:H	3:A:701:TAM:H31	1.71	0.56
1:A:363:GLY:H	3:A:701:TAM:C3	2.19	0.56
1:A:361:ALA:CB	3:A:701:TAM:C6	2.82	0.56
1:A:285:LEU:HG	1:A:289:LEU:HD22	1.89	0.55
1:A:361:ALA:HB3	3:A:701:TAM:C6	2.35	0.55
1:A:194:GLU:OE2	1:A:198:THR:HG21	2.06	0.55
1:A:511:GLY:HA2	1:A:621:PRO:HB2	1.89	0.55
1:A:115:ASP:OD1	1:A:117:ASN:OD1	2.26	0.54
3:A:701:TAM:H62	3:A:701:TAM:C4	2.36	0.54
1:A:510:ILE:HD11	1:A:626:ILE:HG13	1.90	0.53
1:A:227:ASP:HB3	1:A:229:TYR:CE2	2.44	0.53
1:A:413:HIS:CD2	3:A:701:TAM:H11	2.44	0.52
1:A:254:GLY:HA3	1:A:384:ILE:HA	1.90	0.51
3:A:701:TAM:HN2	2:F:12:THR:HG21	1.75	0.51
1:A:541:TYR:OH	1:A:543:GLU:OE2	2.25	0.50
1:A:200:LEU:HD21	1:A:237:TYR:CE2	2.47	0.50
1:A:280:CYS:HB3	1:A:284:TRP:CD1	2.46	0.49
1:A:200:LEU:HD21	1:A:237:TYR:CD2	2.48	0.48
1:A:495:TYR:HE2	1:A:553:ASN:HB2	1.79	0.47
1:A:249:GLN:OE1	1:A:257:THR:CG2	2.61	0.47
1:A:513:ARG:O	1:A:513:ARG:HG2	2.15	0.47
1:A:413:HIS:CG	3:A:701:TAM:H41	2.49	0.47
1:A:250:LYS:H	1:A:250:LYS:HG3	1.36	0.46
1:A:413:HIS:ND1	3:A:701:TAM:H41	2.31	0.46
1:A:190:VAL:HG12	5:A:717:UDP:O2	2.16	0.45
1:A:364:LEU:H	3:A:701:TAM:HO6	1.65	0.44
1:A:528:LEU:HD12	1:A:528:LEU:N	2.32	0.44
1:A:363:GLY:H	3:A:701:TAM:C6	2.30	0.44
1:A:561:HIS:ND1	1:A:585:GLU:OE2	2.44	0.44
3:A:701:TAM:HN2	2:F:12:THR:HB	1.83	0.43
1:A:391:GLU:OE2	1:A:395:ARG:HD3	2.19	0.43
3:A:701:TAM:HN2	2:F:12:THR:CG2	2.30	0.43
1:A:303:ASP:HB2	1:A:407:PRO:HA	2.00	0.43
1:A:129:ILE:HD13	1:A:130:ASN:ND2	2.33	0.43
1:A:295:ASN:HD21	1:A:402:GLN:NE2	2.16	0.43
1:A:187:ILE:HD13	1:A:272:THR:HB	2.00	0.43
3:A:701:TAM:H22	5:A:717:UDP:PB	2.59	0.43
1:A:119:PRO:HB3	1:A:126:PHE:CD1	2.54	0.43
1:A:361:ALA:HB1	3:A:701:TAM:C6	2.49	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:701:TAM:N	2:F:12:THR:HB	2.35	0.41
1:A:168:PRO:HG2	1:A:351:GLU:HG3	2.02	0.41
1:A:218:ILE:HB	1:A:244:VAL:HG22	2.03	0.41
1:A:385:TRP:CZ3	2:F:10:GLY:HA2	2.56	0.41
1:A:557:GLU:HG2	1:A:572:CYS:HB2	2.03	0.41
1:A:451:ARG:HG2	1:A:541:TYR:CE1	2.55	0.41
3:A:701:TAM:N	2:F:12:THR:HG21	2.36	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	535/631 (85%)	510 (95%)	22 (4%)	3 (1%)	25	20
2	F	12/14 (86%)	7 (58%)	3 (25%)	2 (17%)	0	0
All	All	547/645 (85%)	517 (94%)	25 (5%)	5 (1%)	17	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	GLY
1	A	377	SER
2	F	6	GLY
1	A	577	GLN
2	F	7	ALA

### 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	474/556 (85%)	450 (95%)	24 (5%)	24	21
2	F	5/5 (100%)	5 (100%)	0	100	100
All	All	479/561 (85%)	455 (95%)	24 (5%)	24	22

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	CYS
1	A	113	LEU
1	A	130	ASN
1	A	133	SER
1	A	137	LYS
1	A	185	THR
1	A	198	THR
1	A	249	GLN
1	A	250	LYS
1	A	289	LEU
1	A	322	HIS
1	A	342	LYS
1	A	360	PHE
1	A	380	GLU
1	A	417	SER
1	A	425	LYS
1	A	429	VAL
1	A	437	LEU
1	A	502	LEU
1	A	570	ARG
1	A	578	LYS
1	A	590	GLN
1	A	607	ASN
1	A	627	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	GLN
1	A	130	ASN
1	A	140	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	231	HIS
1	A	402	GLN
1	A	547	HIS
1	A	577	GLN
1	A	589	HIS
1	A	597	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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	PO4	A	705	-	4,4,4	0.75	0	6,6,6	0.40	0
4	PO4	F	102	-	4,4,4	0.80	0	6,6,6	0.53	0
4	PO4	A	713	-	4,4,4	1.02	0	6,6,6	0.37	0
4	PO4	A	706	-	4,4,4	1.31	1 (25%)	6,6,6	0.45	0
4	PO4	A	708	-	4,4,4	0.77	0	6,6,6	0.51	0
4	PO4	A	711	-	4,4,4	0.40	0	6,6,6	0.62	0
4	PO4	A	704	-	4,4,4	0.78	0	6,6,6	0.41	0
4	PO4	A	714	-	4,4,4	0.79	0	6,6,6	0.36	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NGA	F	101	2	14,14,15	0.64	0	17,19,21	1.18	2 (11%)
3	TAM	A	701	-	7,10,10	0.58	0	9,12,12	0.43	0
4	PO4	A	707	-	4,4,4	1.12	0	6,6,6	0.35	0
4	PO4	A	716	-	4,4,4	0.81	0	6,6,6	0.39	0
4	PO4	A	703	-	4,4,4	1.01	0	6,6,6	0.52	0
4	PO4	A	710	-	4,4,4	0.73	0	6,6,6	0.43	0
5	UDP	A	717	6	24,26,26	1.32	5 (20%)	37,40,40	1.80	7 (18%)
4	PO4	A	712	-	4,4,4	0.76	0	6,6,6	0.55	0
4	PO4	A	702	-	4,4,4	0.55	0	6,6,6	0.46	0
4	PO4	A	715	-	4,4,4	0.54	0	6,6,6	0.54	0
7	NAG	A	719	1	14,14,15	0.27	0	17,19,21	1.54	3 (17%)
4	PO4	A	709	-	4,4,4	0.61	0	6,6,6	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	UDP	A	717	6	-	1/16/32/32	0/2/2/2
8	NGA	F	101	2	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	A	719	1	-	1/6/23/26	0/1/1/1
3	TAM	A	701	-	-	12/12/12/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	717	UDP	C2-N3	-2.83	1.32	1.38
5	A	717	UDP	C4-N3	-2.39	1.34	1.38
5	A	717	UDP	C6-C5	2.29	1.40	1.35
5	A	717	UDP	C6-N1	-2.27	1.32	1.38
4	A	706	PO4	P-O1	2.23	1.56	1.50
5	A	717	UDP	C2-N1	2.05	1.41	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	717	UDP	N3-C2-N1	5.36	122.00	114.89
5	A	717	UDP	C4-N3-C2	-5.12	119.83	126.58
7	A	719	NAG	O5-C5-C6	3.94	113.38	107.20
5	A	717	UDP	C5-C4-N3	3.59	120.21	114.84

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	101	NGA	O5-C1-C2	-3.16	106.30	111.29
7	A	719	NAG	C1-C2-N2	-3.05	105.27	110.49
5	A	717	UDP	O2B-PB-O1B	2.84	121.81	110.68
5	A	717	UDP	O4-C4-C5	-2.60	120.58	125.16
5	A	717	UDP	O2-C2-N3	-2.43	116.98	121.50
8	F	101	NGA	C2-N2-C7	2.36	126.27	122.90
7	A	719	NAG	C8-C7-N2	-2.18	112.41	116.10
5	A	717	UDP	PA-O3A-PB	-2.11	125.57	132.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	F	101	NGA	C1

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	TAM	C2-C-C1-C4
3	A	701	TAM	C3-C-C1-C4
3	A	701	TAM	N-C-C1-C4
3	A	701	TAM	C1-C-C2-C5
3	A	701	TAM	C3-C-C2-C5
3	A	701	TAM	N-C-C2-C5
3	A	701	TAM	N-C-C3-C6
3	A	701	TAM	C-C1-C4-O4
3	A	701	TAM	C1-C-C3-C6
3	A	701	TAM	C-C2-C5-O5
3	A	701	TAM	C-C3-C6-O6
7	A	719	NAG	O5-C5-C6-O6
3	A	701	TAM	C2-C-C3-C6
5	A	717	UDP	C4'-C5'-O5'-PA

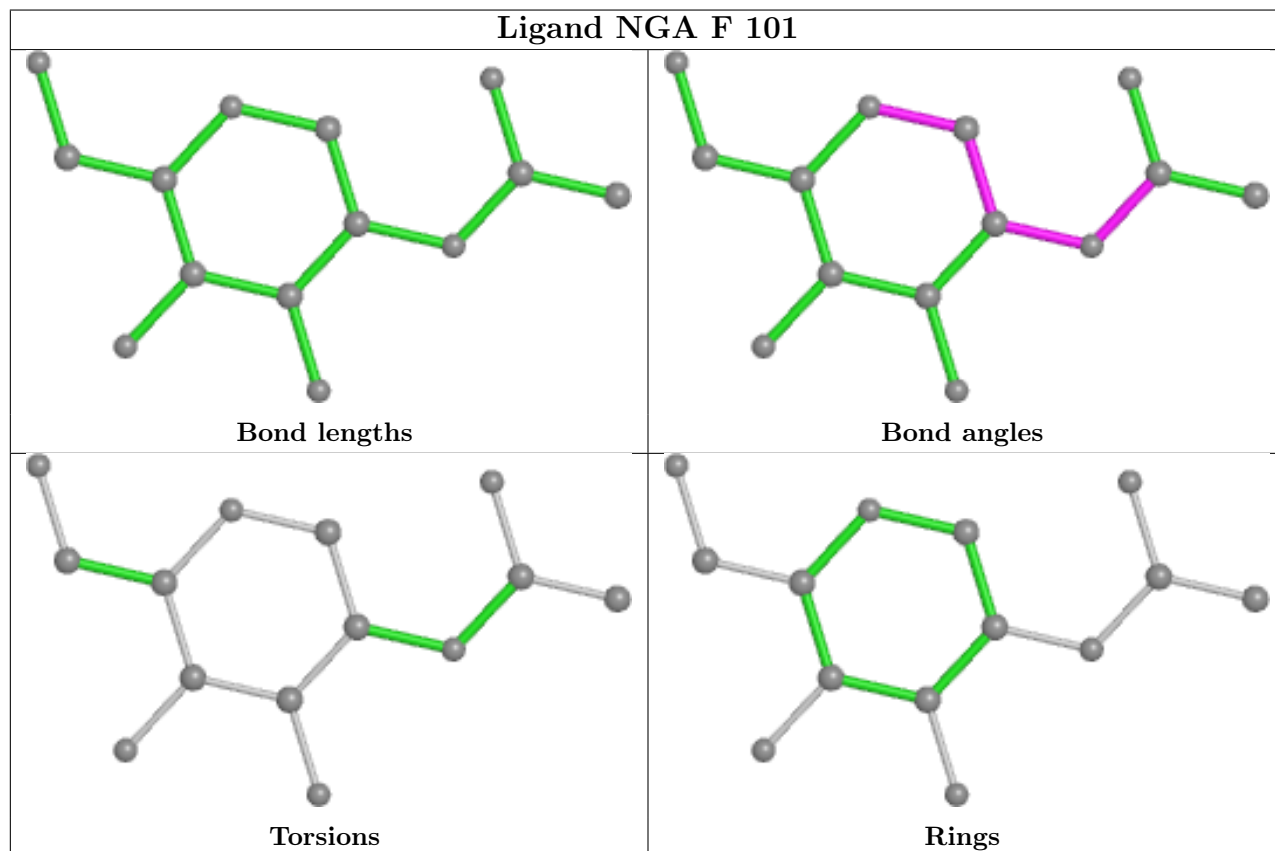
There are no ring outliers.

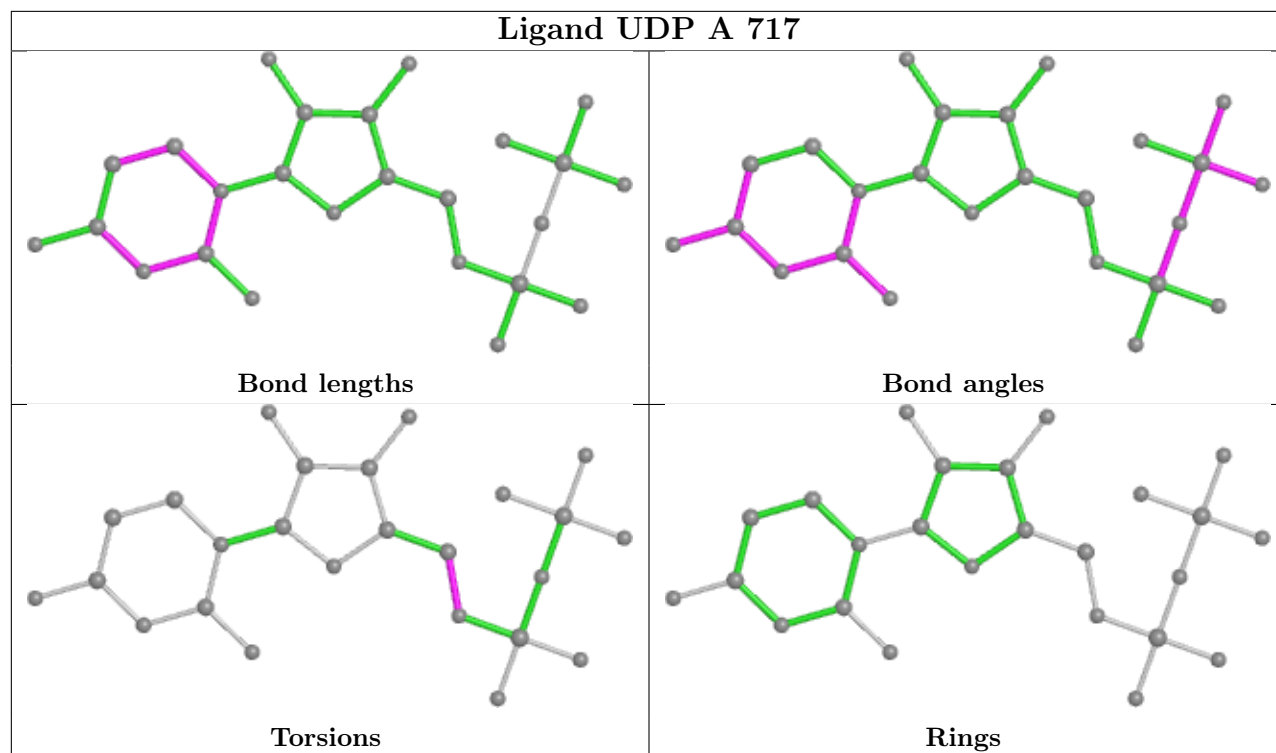
3 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	706	PO4	1	0
3	A	701	TAM	30	0
5	A	717	UDP	4	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	537/631 (85%)	0.26	41 (7%) <b>13</b> <b>17</b>	25, 39, 75, 142	0
2	F	14/14 (100%)	2.45	7 (50%) <b>0</b> <b>0</b>	43, 72, 122, 135	0
All	All	551/645 (85%)	0.31	48 (8%) <b>10</b> <b>12</b>	25, 39, 79, 142	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	575	LYS	14.0
1	A	576	GLY	11.0
2	F	7	ALA	10.7
1	A	577	GLN	9.8
1	A	574	TYR	6.9
2	F	8	GLY	6.6
1	A	523	HIS	6.1
1	A	579	THR	5.6
1	A	129	ILE	5.4
1	A	578	LYS	5.3
1	A	580	PHE	5.0
1	A	320	TYR	4.8
1	A	322	HIS	4.7
2	F	6	GLY	4.5
1	A	323	SER	4.4
1	A	140	GLN	4.2
1	A	520	GLU	4.2
1	A	130	ASN	4.1
1	A	425	LYS	3.9
1	A	94	HIS	3.8
1	A	424	PRO	3.7
1	A	133	SER	3.5
2	F	9	ALA	3.3
1	A	321	GLY	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	F	2	ALA	3.2
1	A	134	GLU	3.1
2	F	4	GLY	3.1
1	A	608	GLY	3.0
1	A	342	LYS	2.9
1	A	131	LEU	2.8
1	A	560	LEU	2.8
1	A	405	ILE	2.7
1	A	251	GLU	2.7
1	A	343	HIS	2.7
1	A	521	ASN	2.7
1	A	144	GLU	2.6
1	A	564	LYS	2.5
1	A	346	LYS	2.3
2	F	5	ALA	2.3
1	A	426	GLY	2.3
1	A	573	THR	2.2
1	A	609	GLU	2.2
1	A	524	GLY	2.2
1	A	550	ILE	2.2
1	A	542	PHE	2.1
1	A	604	LEU	2.0
1	A	417	SER	2.0
1	A	307	ILE	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](#)

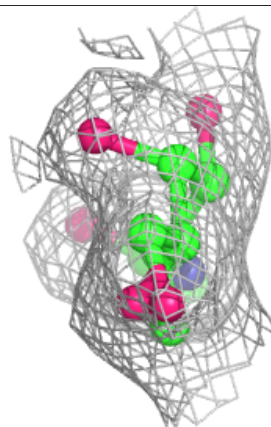
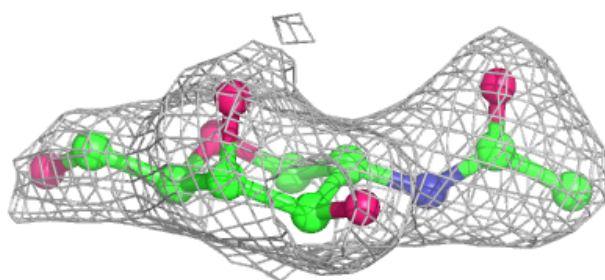
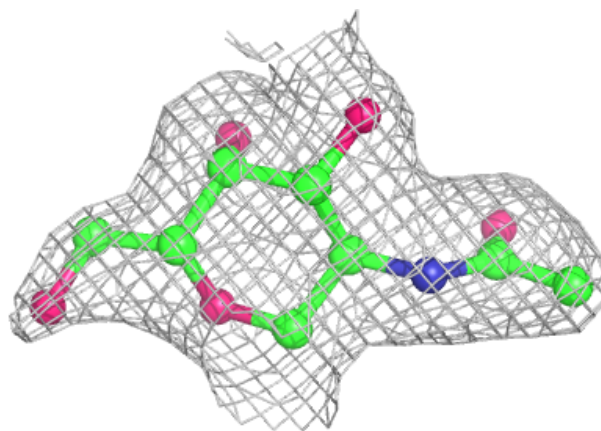
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PO4	A	704	5/5	0.74	0.65	100,126,137,139	0
4	PO4	A	711	5/5	0.75	0.25	81,84,98,104	0
4	PO4	A	715	5/5	0.75	0.41	69,77,91,93	0
4	PO4	A	709	5/5	0.83	0.24	78,92,107,107	0
4	PO4	A	708	5/5	0.85	0.24	66,79,88,90	0
3	TAM	A	701	11/11	0.85	0.27	49,61,70,75	0
7	NAG	A	719	14/15	0.89	0.25	59,69,76,77	0
4	PO4	A	705	5/5	0.91	0.40	80,80,90,97	0
4	PO4	A	703	5/5	0.91	0.14	49,66,69,75	0
8	NGA	F	101	14/15	0.91	0.12	40,43,52,60	0
4	PO4	A	707	5/5	0.92	0.16	54,61,77,78	0
4	PO4	A	713	5/5	0.94	0.14	55,64,66,68	0
4	PO4	A	714	5/5	0.94	0.32	80,84,90,91	0
4	PO4	A	702	5/5	0.94	0.27	79,79,86,88	0
4	PO4	A	716	5/5	0.94	0.30	81,84,88,97	0
4	PO4	F	102	5/5	0.94	0.36	53,66,75,78	0
4	PO4	A	710	5/5	0.94	0.15	67,67,73,82	0
4	PO4	A	706	5/5	0.94	0.13	55,61,65,74	0
4	PO4	A	712	5/5	0.96	0.29	73,78,83,88	0
5	UDP	A	717	25/25	0.96	0.10	37,44,51,54	0
6	MN	A	718	1/1	0.99	0.03	35,35,35,35	0

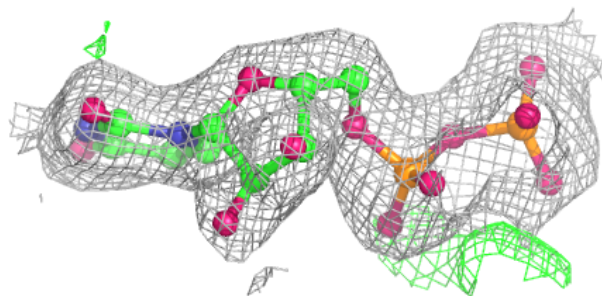
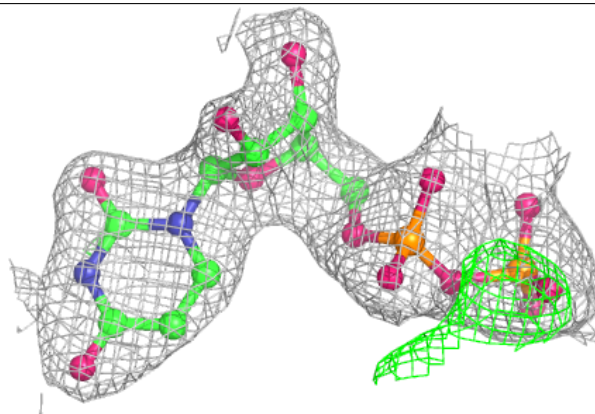
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around NGA F 101:**

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

**Electron density around UDP A 717:**

$2mF_o-DF_c$  (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.