



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:23 PM UTC

PDB ID : 6S24 / pdb_00006s24
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

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)

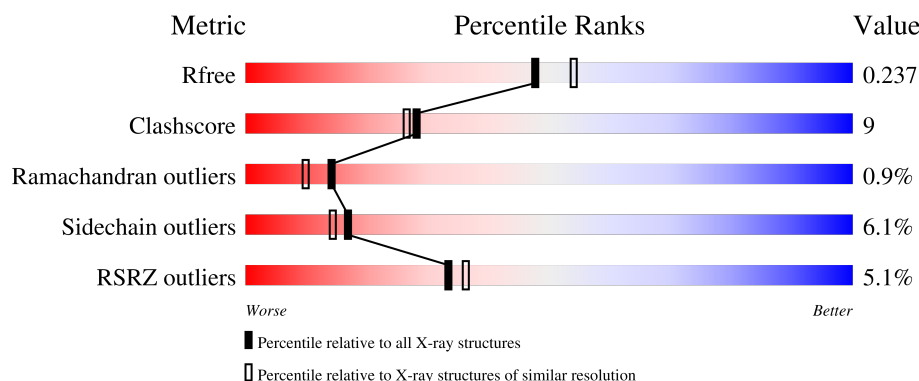
1 Overall quality at a glance

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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 ≥ 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	 3% 69% 14% 15%
2	F	14	 50% 71% 29%

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

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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	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.

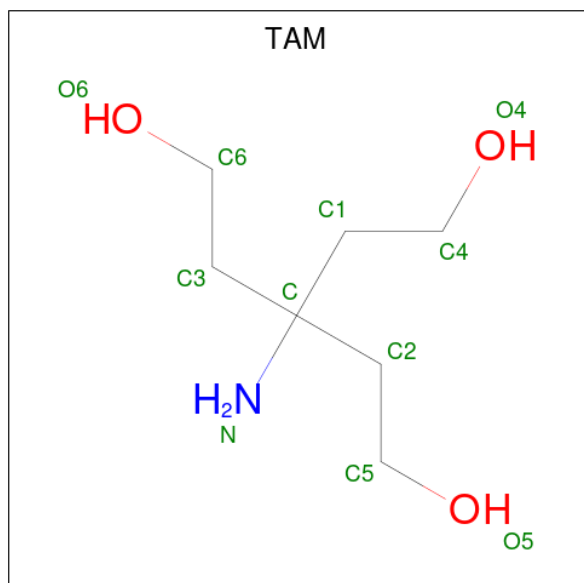
- Molecule 1 is a protein called Polypeptide N-acetylgalactosaminyltransferase.

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-TH R-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 (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).



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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



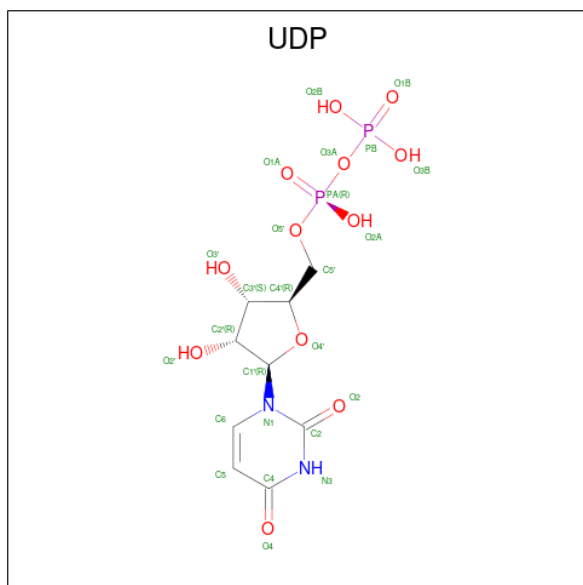
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total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

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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 (CCD ID: 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
			25	9	2	12	2	0

- Molecule 6 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

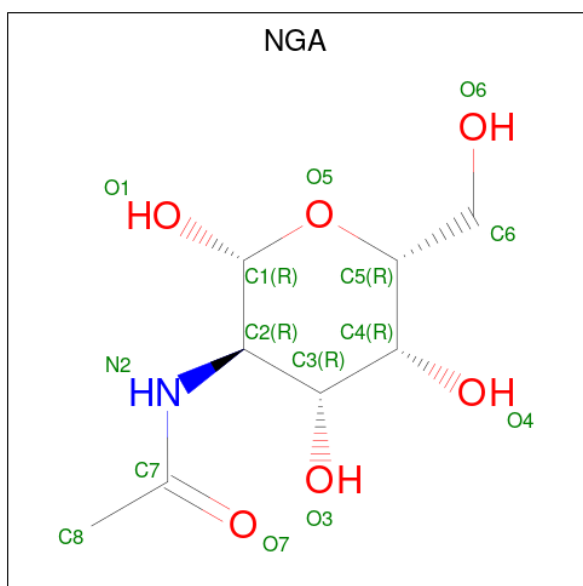
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mn	0	0
			1	1		

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



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

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



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

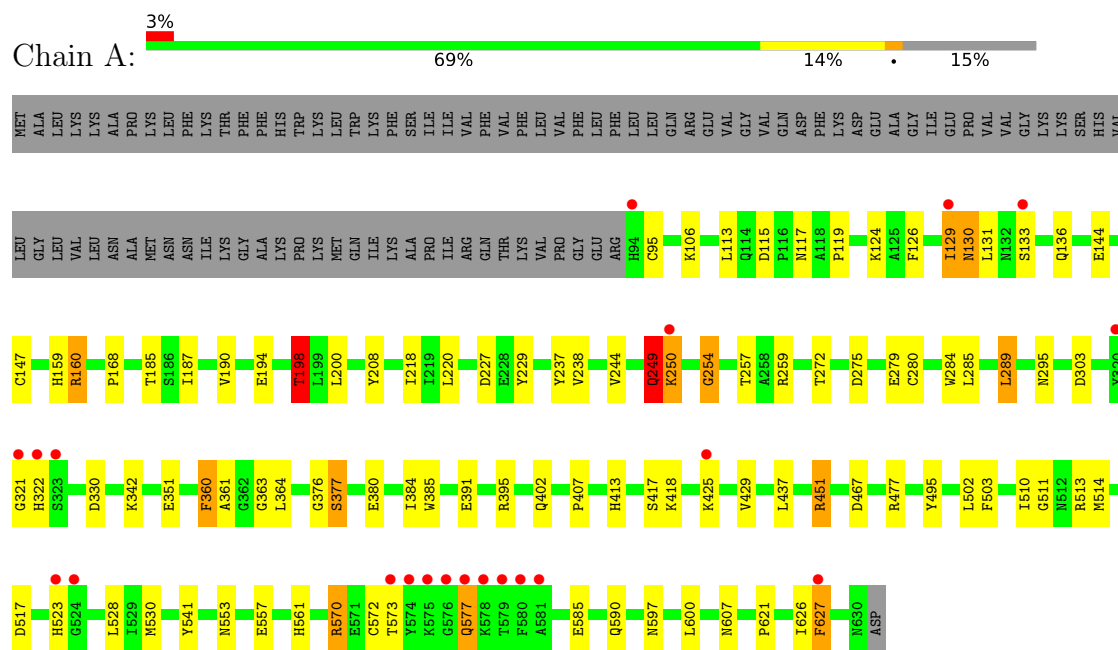
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	200	Total 200	O 200	0	0
9	F	1	Total 1	O 1	0	0

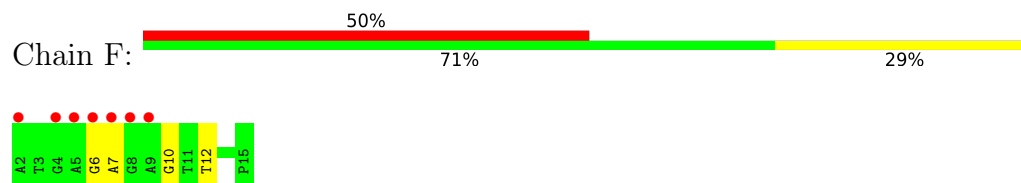
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Polypeptide N-acetylgalactosaminyltransferase



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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) 93.7 (19.96-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.13Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.191 , 0.237 0.199 , 0.237	Depositor DCC
R_{free} test set	1659 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.6	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	0.96	EDS
Total number of atoms	4756	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage'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.*

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: MN, TAM, UDP, NGA, NAG, PO4

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	1.06	2/4456 (0.0%)	1.40	12/6037 (0.2%)
2	F	1.20	0/76	1.45	0/104
All	All	1.07	2/4532 (0.0%)	1.40	12/6141 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	523	HIS	N-CA	5.58	1.51	1.46
1	A	523	HIS	C-O	5.50	1.30	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	THR	CB-CA-C	8.34	124.80	110.79
1	A	249	GLN	CA-C-N	6.38	129.15	120.54
1	A	249	GLN	C-N-CA	6.38	129.15	120.54
1	A	106	LYS	CB-CA-C	6.11	119.01	109.42
1	A	360	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	451	ARG	N-CA-CB	-5.73	101.70	110.12
1	A	160	ARG	CB-CG-CD	5.67	124.34	111.30
1	A	573	THR	CA-CB-OG1	-5.57	101.25	109.60
1	A	198	THR	N-CA-CB	-5.50	101.99	110.13
1	A	254	GLY	CA-C-N	5.41	127.53	120.28
1	A	254	GLY	C-N-CA	5.41	127.53	120.28
1	A	467	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	67	0
2	F	75	0	68	7	0
3	A	11	0	17	30	0
4	A	75	0	0	1	0
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	1	0
9	A	200	0	0	2	0
9	F	1	0	0	0	0
All	All	4756	0	4320	79	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 9.

All (79) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:159:HIS:ND1	1:A:208:TYR:OH	2.43	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:514:MET:HE2	1:A:530:MET:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:376:GLY:O	1:A:377:SER:C	2.60	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:503:PHE:C	1:A:503:PHE:CD1	2.97	0.42
1:A:517:ASP:OD2	8:F:101:NGA:O3	2.35	0.42
1:A:361:ALA:HB1	3:A:701:TAM:C6	2.49	0.41
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
1:A:330:ASP:OD1	1:A:330:ASP:C	2.65	0.40
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%)	21	18
2	F	12/14 (86%)	7 (58%)	3 (25%)	2 (17%)	0	0
All	All	547/645 (85%)	517 (94%)	25 (5%)	5 (1%)	14	10

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 ⓘ

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%)	445 (94%)	29 (6%)	17	14
2	F	5/5 (100%)	5 (100%)	0	100	100
All	All	479/561 (85%)	450 (94%)	29 (6%)	17	14

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	CYS
1	A	113	LEU
1	A	124	LYS
1	A	129	ILE
1	A	130	ASN
1	A	133	SER
1	A	144	GLU
1	A	185	THR
1	A	198	THR
1	A	220	LEU
1	A	238	VAL
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

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Mol	Chain	Res	Type
1	A	417	SER
1	A	418	LYS
1	A	425	LYS
1	A	429	VAL
1	A	437	LEU
1	A	502	LEU
1	A	570	ARG
1	A	577	GLN
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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	140	GLN
1	A	402	GLN
1	A	421	HIS
1	A	428	GLN
1	A	462	GLN
1	A	522	ASN
1	A	577	GLN
1	A	589	HIS
1	A	597	ASN
1	A	601	HIS

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

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	714	-	4,4,4	0.84	0	6,6,6	0.39	0
4	PO4	A	706	-	4,4,4	1.38	1 (25%)	6,6,6	0.47	0
4	PO4	A	710	-	4,4,4	0.78	0	6,6,6	0.46	0
4	PO4	A	713	-	4,4,4	1.07	0	6,6,6	0.39	0
4	PO4	A	711	-	4,4,4	0.44	0	6,6,6	0.66	0
4	PO4	A	705	-	4,4,4	0.80	0	6,6,6	0.43	0
4	PO4	A	707	-	4,4,4	1.18	0	6,6,6	0.37	0
7	NAG	A	719	1	14,14,15	0.27	0	17,19,21	1.44	3 (17%)
4	PO4	A	703	-	4,4,4	1.06	0	6,6,6	0.54	0
3	TAM	A	701	-	10,10,10	0.96	0	12,12,12	2.04	3 (25%)
5	UDP	A	717	6	25,26,26	1.41	6 (24%)	38,40,40	1.88	7 (18%)
4	PO4	A	708	-	4,4,4	0.81	0	6,6,6	0.54	0
4	PO4	A	702	-	4,4,4	0.60	0	6,6,6	0.49	0
4	PO4	F	102	-	4,4,4	0.85	0	6,6,6	0.56	0
4	PO4	A	716	-	4,4,4	0.87	0	6,6,6	0.42	0
4	PO4	A	715	-	4,4,4	0.58	0	6,6,6	0.57	0
4	PO4	A	709	-	4,4,4	0.66	0	6,6,6	0.53	0
4	PO4	A	712	-	4,4,4	0.81	0	6,6,6	0.59	0
8	NGA	F	101	2	14,14,15	0.66	0	17,19,21	1.21	2 (11%)
4	PO4	A	704	-	4,4,4	0.83	0	6,6,6	0.44	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
3	TAM	A	701	-	-	12/12/12/12	-
7	NAG	A	719	1	-	1/6/23/26	0/1/1/1
5	UDP	A	717	6	-	3/16/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NGA	F	101	2	1/1/5/7	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	717	UDP	C2-N3	-2.90	1.32	1.38
5	A	717	UDP	PA-O3A	2.55	1.62	1.59
5	A	717	UDP	C4-N3	-2.54	1.34	1.38
4	A	706	PO4	P-O1	2.34	1.56	1.50
5	A	717	UDP	C6-N1	-2.34	1.32	1.38
5	A	717	UDP	C6-C5	2.27	1.40	1.35
5	A	717	UDP	C2-N1	2.10	1.41	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	717	UDP	C4-N3-C2	-5.46	119.83	126.61
5	A	717	UDP	N3-C2-N1	5.46	122.00	114.89
3	A	701	TAM	C4-C1-C	-4.12	111.11	115.97
3	A	701	TAM	C6-C3-C	-4.10	111.14	115.97
5	A	717	UDP	C5-C4-N3	3.86	120.21	114.80
3	A	701	TAM	C5-C2-C	-3.79	111.49	115.97
7	A	719	NAG	C1-C2-N2	-3.28	105.27	110.43
8	F	101	NGA	O5-C1-C2	-3.22	106.30	111.29
5	A	717	UDP	O2A-PA-O3A	2.94	115.22	107.27
7	A	719	NAG	O5-C5-C6	2.93	113.38	107.66
5	A	717	UDP	O2B-PB-O1B	2.82	121.81	110.83
5	A	717	UDP	O4-C4-C5	-2.66	120.58	125.16
8	F	101	NGA	C2-N2-C7	2.51	126.27	122.90
5	A	717	UDP	O2-C2-N3	-2.45	116.98	121.49
7	A	719	NAG	C8-C7-N2	-2.23	112.41	116.12

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	F	101	NGA	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	TAM	C2-C-C1-C4

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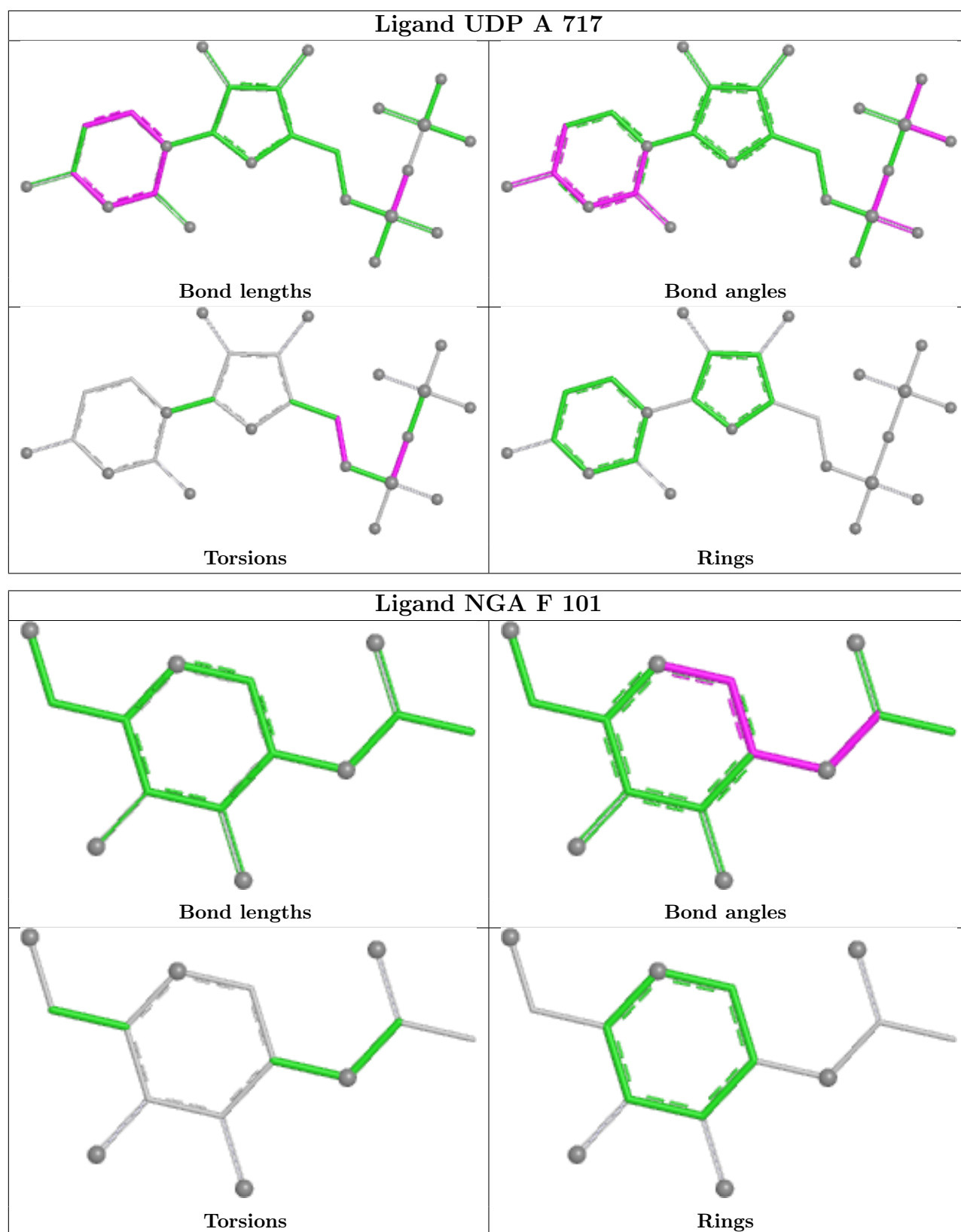
Mol	Chain	Res	Type	Atoms
3	A	701	TAM	C3-C-C1-C4
3	A	701	TAM	N-C-C1-C4
3	A	701	TAM	C1-C-C2-C5
3	A	701	TAM	C3-C-C2-C5
3	A	701	TAM	N-C-C2-C5
3	A	701	TAM	N-C-C3-C6
3	A	701	TAM	C-C1-C4-O4
3	A	701	TAM	C-C2-C5-O5
3	A	701	TAM	C-C3-C6-O6
3	A	701	TAM	C1-C-C3-C6
7	A	719	NAG	O5-C5-C6-O6
3	A	701	TAM	C2-C-C3-C6
5	A	717	UDP	C4'-C5'-O5'-PA
5	A	717	UDP	PB-O3A-PA-O1A
5	A	717	UDP	PB-O3A-PA-O2A

There are no ring outliers.

4 monomers are involved in 33 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
8	F	101	NGA	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	537/631 (85%)	0.02	21 (3%) 43 46	25, 39, 75, 142	0
2	F	14/14 (100%)	2.04	7 (50%) 0 0	43, 72, 122, 135	0
All	All	551/645 (85%)	0.07	28 (5%) 33 36	25, 39, 79, 142	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	580	PHE	5.4
1	A	94	HIS	5.3
1	A	574	TYR	5.0
1	A	524	GLY	4.8
1	A	523	HIS	4.7
2	F	5	ALA	4.6
2	F	7	ALA	4.4
1	A	575	LYS	4.3
2	F	9	ALA	4.2
1	A	581	ALA	4.0
1	A	129	ILE	3.6
1	A	320	TYR	3.5
2	F	6	GLY	3.1
1	A	576	GLY	3.0
2	F	8	GLY	2.9
1	A	425	LYS	2.9
2	F	2	ALA	2.9
2	F	4	GLY	2.8
1	A	573	THR	2.7
1	A	133	SER	2.6
1	A	322	HIS	2.5
1	A	321	GLY	2.4
1	A	578	LYS	2.3
1	A	323	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	577	GLN	2.2
1	A	579	THR	2.2
1	A	250	LYS	2.0
1	A	627	PHE	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.

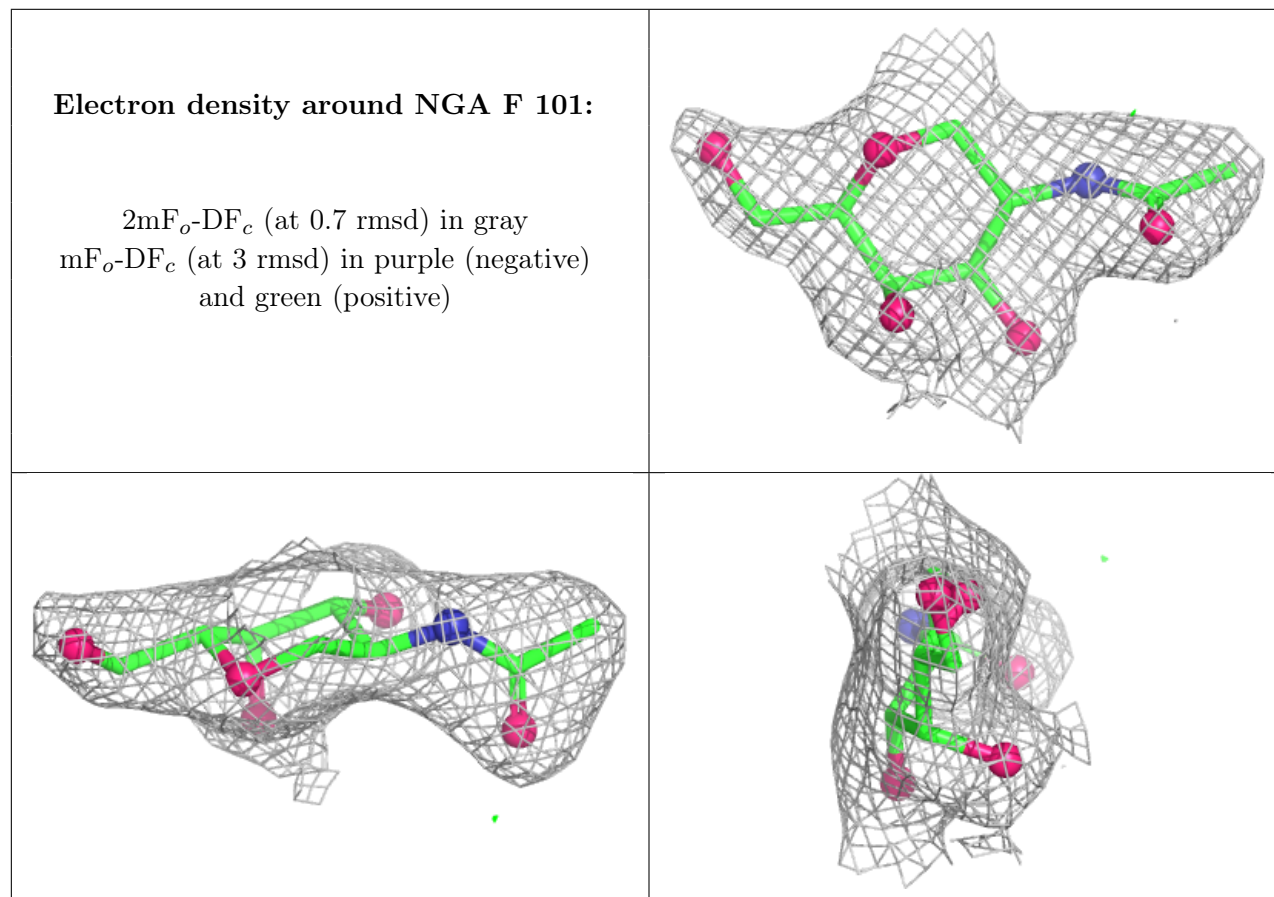
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PO4	A	715	5/5	0.62	0.12	69,77,91,93	0
4	PO4	A	709	5/5	0.73	0.11	78,92,107,107	0
4	PO4	A	708	5/5	0.77	0.11	66,79,88,90	0
4	PO4	A	704	5/5	0.80	0.16	100,126,137,139	0
4	PO4	A	702	5/5	0.81	0.09	79,79,86,88	0
7	NAG	A	719	14/15	0.81	0.11	59,69,76,77	0
4	PO4	A	705	5/5	0.82	0.08	80,80,90,97	0
4	PO4	A	711	5/5	0.82	0.15	81,84,98,104	0
3	TAM	A	701	11/11	0.85	0.20	49,61,70,75	0
4	PO4	A	714	5/5	0.86	0.07	80,84,90,91	0
4	PO4	A	703	5/5	0.88	0.18	49,66,69,75	0
4	PO4	A	707	5/5	0.89	0.12	54,61,77,78	0
4	PO4	A	716	5/5	0.90	0.06	81,84,88,97	0
4	PO4	A	712	5/5	0.90	0.07	73,78,83,88	0
4	PO4	F	102	5/5	0.91	0.20	53,66,75,78	0
4	PO4	A	710	5/5	0.91	0.10	67,67,73,82	0
4	PO4	A	706	5/5	0.93	0.12	55,61,65,74	0
4	PO4	A	713	5/5	0.94	0.12	55,64,66,68	0
8	NGA	F	101	14/15	0.95	0.06	40,43,52,60	0

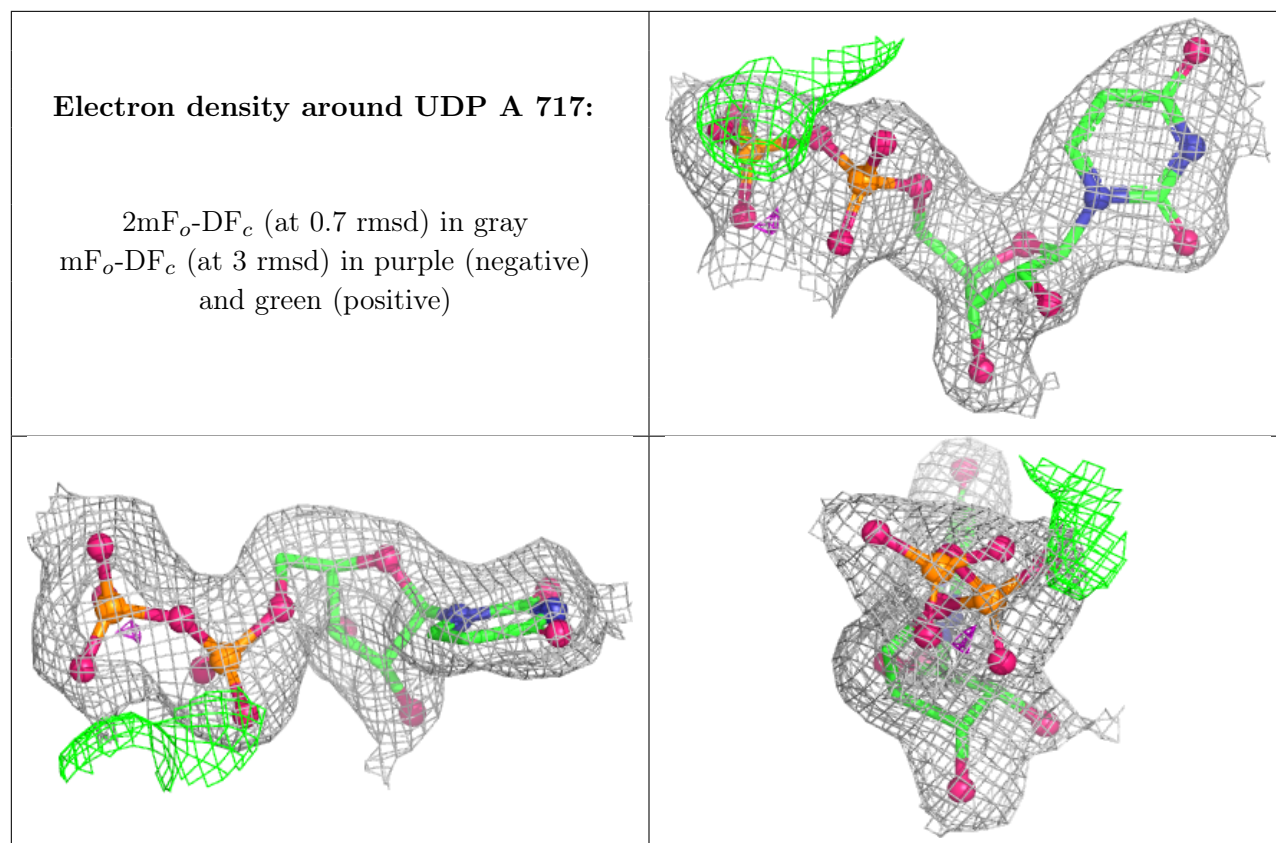
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	UDP	A	717	25/25	0.96	0.06	37,44,51,54	0
6	MN	A	718	1/1	1.00	0.04	35,35,35,35	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.