



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:19 AM UTC

PDB ID : 4GZ3 / pdb_00004gz3
Title : Crystal structure of human O-GlcNAc Transferase with UDP and a thioglycopeptide
Authors : Lazarus, M.B.; Jiang, J.; Gloster, T.M.; Zandberg, W.F.; Vocadlo, D.J.; Walker, S.
Deposited on : 2012-09-05
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

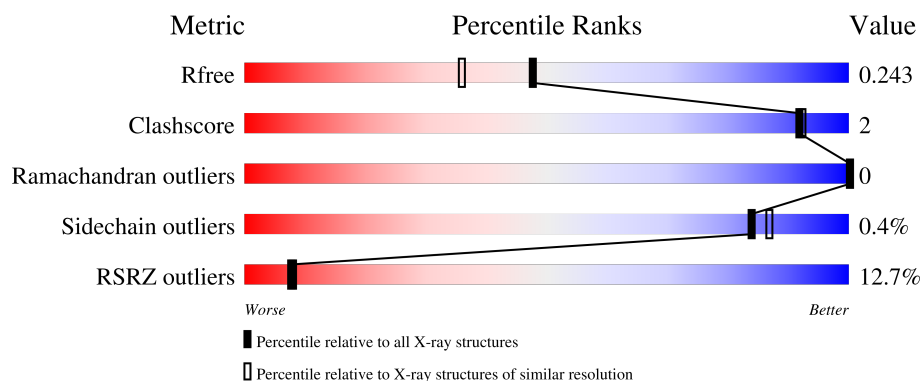
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	723	13% 92% . .
1	C	723	12% 89% . 7%
2	B	14	14% 79% 21%
2	D	14	7% 93% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12010 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 UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	695	Total	C	N	O	S	0	7	0
			5530	3510	966	1017	37			
1	C	674	Total	C	N	O	S	0	6	0
			5361	3413	934	976	38			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	GLY	-	expression tag	UNP O15294
A	310	PRO	-	expression tag	UNP O15294
A	311	GLY	-	expression tag	UNP O15294
A	312	SER	-	expression tag	UNP O15294
C	309	GLY	-	expression tag	UNP O15294
C	310	PRO	-	expression tag	UNP O15294
C	311	GLY	-	expression tag	UNP O15294
C	312	SER	-	expression tag	UNP O15294

- Molecule 2 is a protein called Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	S	0	0	0
			95	58	15	20	2			
2	D	14	Total	C	N	O	S	0	0	0
			95	58	15	20	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	TYR	-	expression tag	UNP P68400
D	13	TYR	-	expression tag	UNP P68400

-
- The diagram illustrates the chemical structure of UDP (Uridine Diphosphate). It consists of a uracil base (a six-membered ring with two nitrogen atoms, N1 and N3) attached to a ribose sugar (a five-membered ring). The ribose sugar is linked to a diphosphate group (two phosphate groups connected by an oxygen atom). The uracil base is labeled with atoms N1, N3, C2, C4, C5, and C6. The ribose sugar is labeled with atoms C1', C2', C3', C4', and C5'. The diphosphate group is labeled with atoms O1A, O1B, O2A, O2B, O3A, and O3B. The structure is shown in a 3D representation with wedged and dashed bonds to indicate stereochemistry.

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

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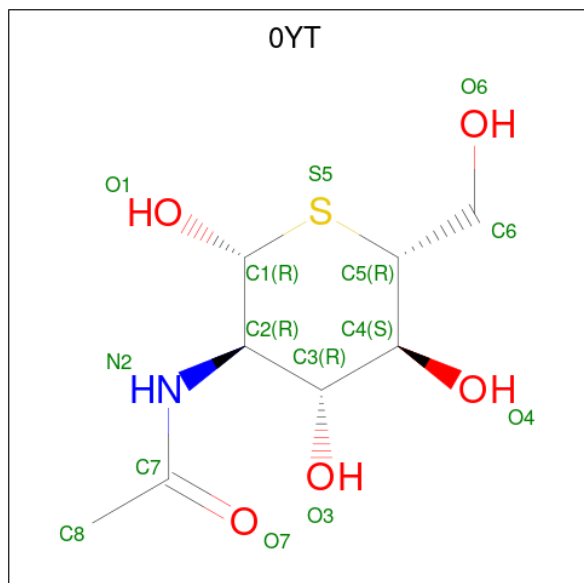
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2-acetamido-2-deoxy-5-thio-beta-D-glucopyranose (CCD ID: 0YT) (formula: $C_8H_{15}NO_5S$).



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

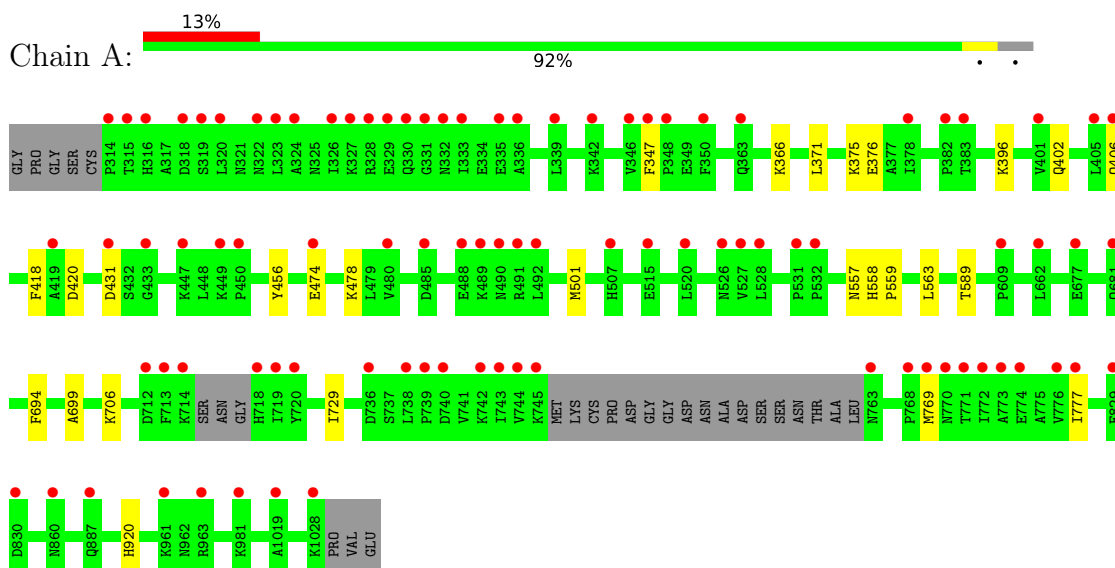
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	419	Total	O	0	0
			419	419		
6	B	8	Total	O	0	0
			8	8		
6	C	397	Total	O	0	0
			397	397		
6	D	12	Total	O	0	0
			12	12		

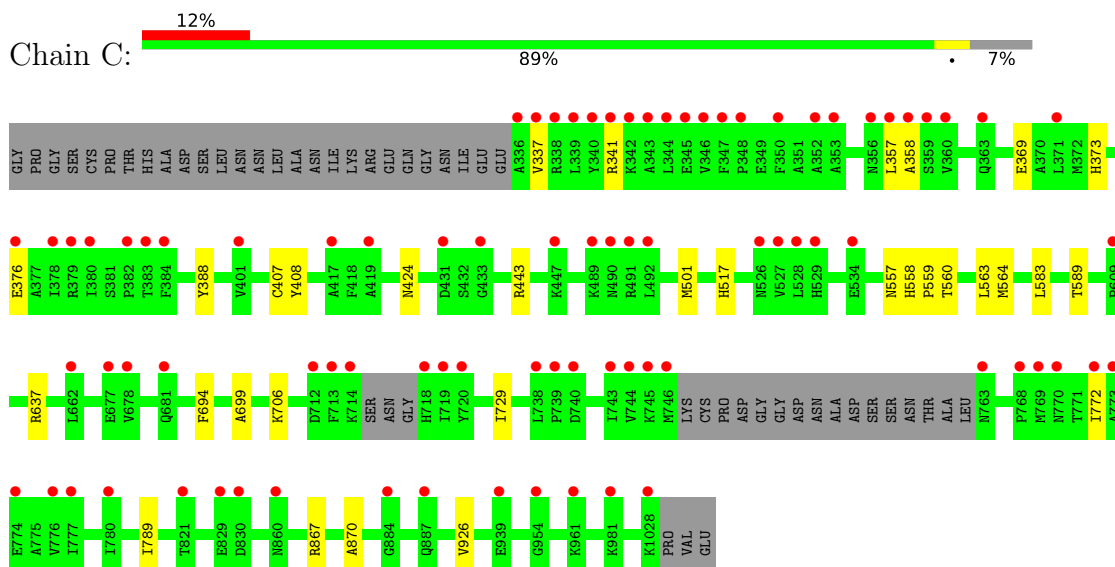
3 Residue-property plots

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.

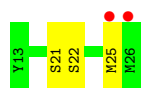
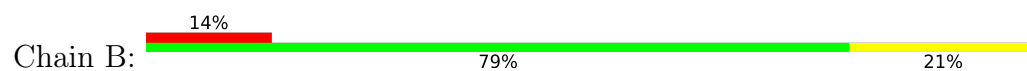
- Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit



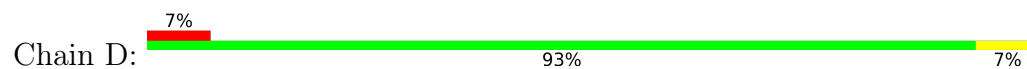
- Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit



- Molecule 2: Casein kinase II subunit alpha



- Molecule 2: Casein kinase II subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.77Å 137.62Å 153.02Å 90.00° 102.82° 90.00°	Depositor
Resolution (Å)	48.15 – 1.90 48.15 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.15-1.90) 98.9 (48.15-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.226 , 0.250 0.221 , 0.243	Depositor DCC
R_{free} test set	7783 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12010	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.18 % 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 9.1973e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 0YT, UDP, SO4

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	0.36	0/5679	0.71	2/7701 (0.0%)
1	C	0.36	0/5506	0.70	0/7466
2	B	0.45	0/97	0.65	0/131
2	D	0.41	0/97	0.73	0/131
All	All	0.36	0/11379	0.70	2/15429 (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	A	347	PHE	CA-C-N	5.14	124.94	119.28
1	A	347	PHE	C-N-CA	5.14	124.94	119.28

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	5530	0	5514	16	0
1	C	5361	0	5357	18	0
2	B	95	0	87	1	0
2	D	95	0	87	0	0
3	A	25	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	25	0	11	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
5	B	14	0	13	2	0
5	D	14	0	13	2	0
6	A	419	0	0	4	0
6	B	8	0	0	1	0
6	C	397	0	0	4	0
6	D	12	0	0	0	0
All	All	12010	0	11093	35	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 2.

All (35) 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:563:LEU:HD12	5:D:101:0YT:H13	1.70	0.74
1:A:563:LEU:HD12	5:B:101:0YT:H13	1.73	0.71
1:C:517:HIS:NE2	6:C:1533:HOH:O	2.30	0.64
1:C:501:MET:HE1	5:D:101:0YT:H5	1.85	0.56
1:A:396:LYS:NZ	1:A:431:ASP:OD2	2.38	0.56
1:A:376:GLU:HG2	6:A:1421:HOH:O	2.05	0.55
1:A:366:LYS:NZ	6:A:1411:HOH:O	2.38	0.55
1:C:376:GLU:HG2	6:C:1351:HOH:O	2.08	0.54
1:A:501:MET:HE1	5:B:101:0YT:H5	1.91	0.53
1:A:558:HIS:CG	1:A:559:PRO:HD2	2.49	0.48
1:C:557:ASN:HB2	1:C:589:THR:HG21	1.97	0.47
1:C:341:ARG:NH2	1:C:369:GLU:OE2	2.40	0.46
1:C:358:ALA:HB2	1:C:373:HIS:HB2	1.98	0.46
1:C:337:VAL:HG13	1:C:357:LEU:HD11	1.98	0.45
1:C:729:ILE:HG13	6:C:1447:HOH:O	2.17	0.45
1:C:699:ALA:O	1:C:706:LYS:NZ	2.50	0.45
1:A:694:PHE:CZ	1:A:920:HIS:HB3	2.53	0.44
1:C:443:ARG:NH2	6:C:1577:HOH:O	2.38	0.43
1:A:418:PHE:CE1	1:A:420:ASP:HB2	2.54	0.43
1:C:558:HIS:CG	1:C:559:PRO:HD2	2.53	0.43
1:A:474:GLU:HG3	6:A:1523:HOH:O	2.19	0.43
1:A:402:GLN:O	1:A:406:GLN:HG2	2.19	0.43
1:C:583:LEU:HD22	1:C:637:ARG:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:SER:HA	6:B:204:HOH:O	2.20	0.42
1:A:729:ILE:HG13	6:A:1390:HOH:O	2.19	0.42
1:C:772:ILE:HG23	1:C:789:ILE:HD13	2.02	0.41
1:A:456:TYR:CZ	1:A:478:LYS:HD3	2.55	0.41
1:A:371:LEU:HG	1:A:375:LYS:HE3	2.02	0.41
1:A:557:ASN:HB2	1:A:589:THR:HG21	2.03	0.41
1:A:769:MET:HE1	1:A:777:ILE:HD12	2.03	0.41
1:C:867:ARG:HB3	1:C:870:ALA:HA	2.03	0.41
1:C:388:TYR:O	1:C:407:CYS:HB3	2.21	0.40
1:C:408:TYR:CZ	1:C:424:ASN:HB3	2.56	0.40
1:A:699:ALA:O	1:A:706:LYS:NZ	2.54	0.40
1:C:560:THR:O	1:C:564:MET:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	697/723 (96%)	684 (98%)	13 (2%)	0	100	100
1	C	674/723 (93%)	662 (98%)	12 (2%)	0	100	100
2	B	12/14 (86%)	12 (100%)	0	0	100	100
2	D	12/14 (86%)	12 (100%)	0	0	100	100
All	All	1395/1474 (95%)	1370 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	605/618 (98%)	605 (100%)	0	100	100
1	C	585/618 (95%)	583 (100%)	2 (0%)	86	88
2	B	11/11 (100%)	9 (82%)	2 (18%)	2	0
2	D	11/11 (100%)	10 (91%)	1 (9%)	9	3
All	All	1212/1258 (96%)	1207 (100%)	5 (0%)	84	87

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

Mol	Chain	Res	Type
2	B	22	SER
2	B	25	MET
1	C	694	PHE
1	C	926	VAL
2	D	25	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	519	ASN
1	A	529	HIS
1	A	763	ASN
1	A	802	GLN
1	A	849	GLN
1	A	888	ASN
1	A	964	GLN
1	C	364	GLN
1	C	368	GLN
1	C	802	GLN
1	C	805	ASN
1	C	849	GLN
1	C	878	GLN

5.3.3 RNA ⓘ

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](#)

7 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	$\# Z > 2$
4	SO4	D	102	-	4,4,4	0.26	0	6,6,6	0.18	0
4	SO4	B	102	-	4,4,4	0.24	0	6,6,6	0.05	0
4	SO4	A	1102	-	4,4,4	0.27	0	6,6,6	0.06	0
3	UDP	C	1101	-	25,26,26	1.06	2 (8%)	38,40,40	1.62	5 (13%)
5	0YT	B	101	2	12,14,15	1.30	1 (8%)	12,19,21	1.34	2 (16%)
3	UDP	A	1101	-	25,26,26	1.08	1 (4%)	38,40,40	1.47	5 (13%)
5	0YT	D	101	2	12,14,15	1.27	0	12,19,21	1.32	2 (16%)

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	UDP	A	1101	-	-	3/16/32/32	0/2/2/2
5	0YT	D	101	2	-	2/6/23/26	0/1/1/1
3	UDP	C	1101	-	-	3/16/32/32	0/2/2/2
5	0YT	B	101	2	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1101	UDP	PA-O3A	2.23	1.61	1.59
3	A	1101	UDP	PA-O3A	2.21	1.61	1.59
5	B	101	0YT	O4-C4	-2.04	1.37	1.43
3	C	1101	UDP	C5-C4	-2.01	1.39	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1101	UDP	C4-N3-C2	-5.78	119.43	126.61
3	A	1101	UDP	C4-N3-C2	-5.10	120.28	126.61
3	C	1101	UDP	C5-C4-N3	4.08	120.52	114.80
3	A	1101	UDP	C5-C4-N3	3.99	120.39	114.80
3	C	1101	UDP	N3-C2-N1	3.94	120.03	114.89
3	C	1101	UDP	O4-C4-C5	-3.36	119.37	125.16
3	A	1101	UDP	N3-C2-N1	3.35	119.25	114.89
5	B	101	0YT	C4-C3-C2	3.08	115.53	111.02
3	A	1101	UDP	O4-C4-C5	-3.06	119.88	125.16
5	D	101	0YT	C4-C3-C2	2.97	115.36	111.02
5	D	101	0YT	O6-C6-C5	2.82	117.13	110.72
3	C	1101	UDP	O2-C2-N1	-2.76	119.21	122.80
5	B	101	0YT	O6-C6-C5	2.68	116.80	110.72
3	A	1101	UDP	O2-C2-N1	-2.28	119.83	122.80

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	UDP	PA-O3A-PB-O3B
3	C	1101	UDP	PA-O3A-PB-O3B
5	D	101	0YT	C4-C5-C6-O6
5	D	101	0YT	S5-C5-C6-O6
3	A	1101	UDP	C3'-C4'-C5'-O5'
3	C	1101	UDP	C3'-C4'-C5'-O5'
3	A	1101	UDP	O4'-C4'-C5'-O5'
3	C	1101	UDP	O4'-C4'-C5'-O5'
5	B	101	0YT	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

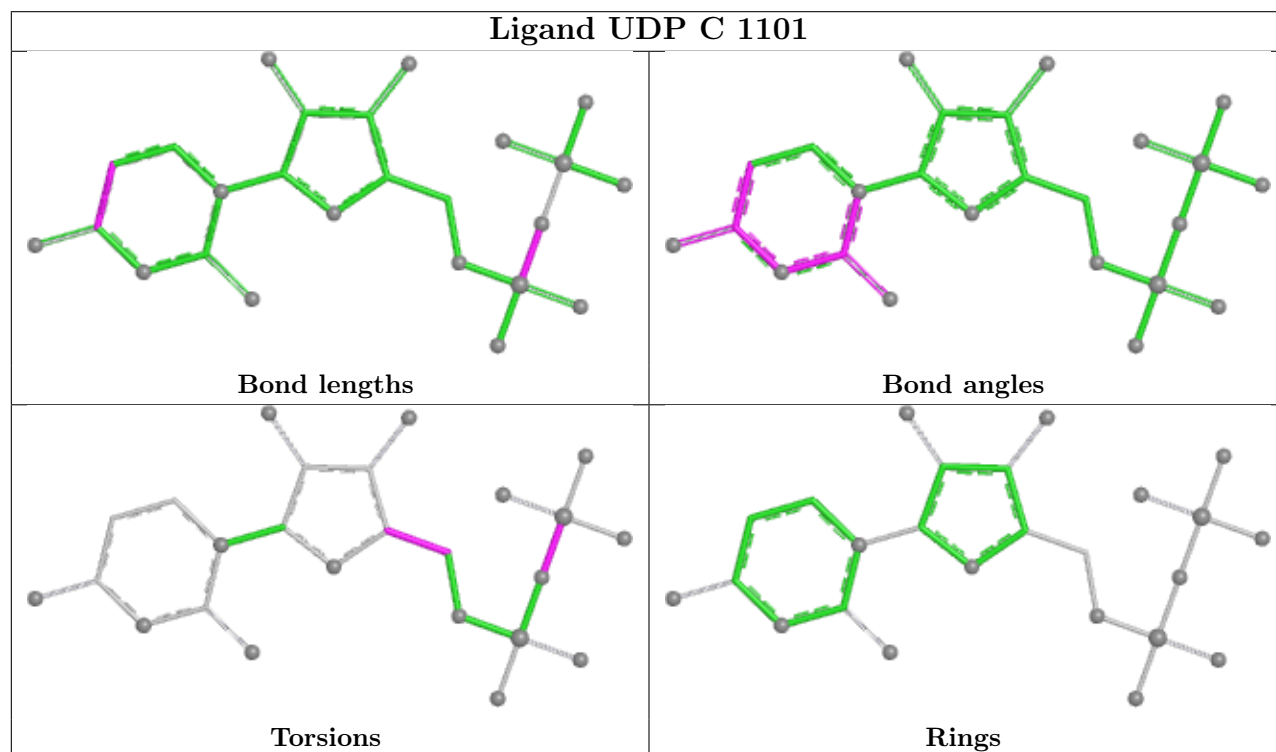
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	101	0YT	2	0

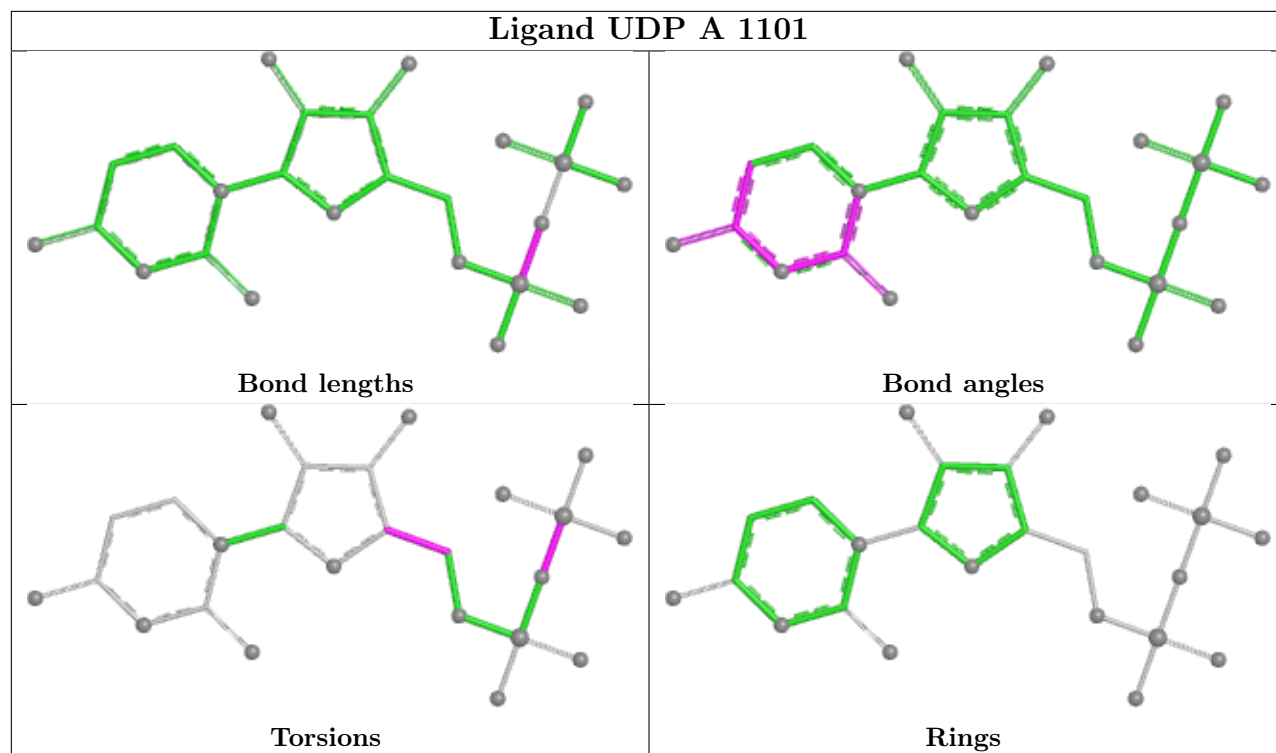
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	101	0YT	2	0

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, 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	695/723 (96%)	0.74	91 (13%) 7 7	10, 25, 54, 92	7 (1%)
1	C	674/723 (93%)	0.69	84 (12%) 8 8	10, 24, 54, 95	6 (0%)
2	B	14/14 (100%)	0.65	2 (14%) 6 6	15, 23, 58, 58	0
2	D	14/14 (100%)	0.38	1 (7%) 22 23	16, 24, 54, 55	0
All	All	1397/1474 (94%)	0.71	178 (12%) 8 8	10, 24, 54, 95	13 (0%)

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	718	HIS	7.9
1	C	339	LEU	7.8
1	A	772	ILE	7.4
1	A	718	HIS	7.3
1	A	713	PHE	7.2
1	A	714	LYS	7.0
1	C	336	ALA	6.9
1	C	713	PHE	6.6
1	A	314	PRO	6.4
1	A	769	MET	6.3
1	A	770	ASN	6.2
1	C	714	LYS	5.9
1	C	346	VAL	5.8
1	C	348	PRO	5.6
1	A	719	ILE	5.6
1	C	772	ILE	5.5
1	A	740	ASP	5.5
1	C	343	ALA	5.3
1	C	719	ILE	5.0
1	C	347	PHE	4.9
1	C	337	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	383	THR	4.8
1	A	763	ASN	4.7
1	C	340	TYR	4.5
1	A	323	LEU	4.5
1	C	344	LEU	4.4
1	A	774	GLU	4.3
1	C	342	LYS	4.2
1	A	489	LYS	4.2
1	A	315	THR	4.2
1	A	830	ASP	4.2
1	C	777	ILE	4.1
1	A	681	GLN	4.0
1	A	347	PHE	4.0
1	A	743	ILE	4.0
1	C	746	MET	4.0
1	C	720	TYR	4.0
1	C	740	ASP	4.0
1	A	720	TYR	3.9
1	C	830	ASP	3.9
1	A	527	VAL	3.9
1	C	350	PHE	3.9
1	A	745	LYS	3.9
1	C	744	VAL	3.9
1	C	359	SER	3.9
1	A	771	THR	3.8
1	C	770	ASN	3.8
1	A	326	ILE	3.8
1	C	763	ASN	3.7
1	C	352	ALA	3.7
1	A	492	LEU	3.7
1	A	744	VAL	3.7
1	C	1028	LYS	3.7
1	C	527	VAL	3.7
1	C	401	VAL	3.6
1	C	382	PRO	3.6
1	A	346	VAL	3.6
1	A	507	HIS	3.6
2	B	25	MET	3.5
1	A	431	ASP	3.5
1	A	447	LYS	3.5
1	C	769	MET	3.5
1	C	743	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	328	ARG	3.4
1	C	829	GLU	3.4
1	A	348	PRO	3.4
1	C	447	LYS	3.3
1	A	331	GLY	3.3
1	C	860	ASN	3.3
1	A	739	PRO	3.3
1	A	526	ASN	3.3
1	C	353	ALA	3.3
1	C	341	ARG	3.3
1	C	433	GLY	3.3
1	A	860	ASN	3.3
1	C	712	ASP	3.2
1	C	360	VAL	3.2
1	C	773	ALA	3.1
1	A	490	ASN	3.1
1	A	324	ALA	3.1
1	A	383	THR	3.1
1	C	417	ALA	3.1
1	A	777	ILE	3.0
1	A	433	GLY	3.0
1	C	745	LYS	3.0
1	A	829	GLU	3.0
2	D	25	MET	3.0
1	C	378	ILE	3.0
1	C	528	LEU	3.0
1	C	526	ASN	3.0
1	C	431	ASP	2.9
1	C	358	ALA	2.9
1	A	742	LYS	2.9
1	C	609	PRO	2.9
1	A	773	ALA	2.9
1	A	335	GLU	2.9
1	A	401	VAL	2.8
1	C	887	GLN	2.8
1	A	378	ILE	2.8
1	C	662	LEU	2.8
1	A	768	PRO	2.8
1	A	485	ASP	2.8
1	A	319[A]	SER	2.8
1	C	529	HIS	2.8
1	A	491	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	887	GLN	2.7
1	A	382	PRO	2.7
1	C	380	ILE	2.7
1	C	491	ARG	2.7
1	A	318	ASP	2.7
1	C	357	LEU	2.7
1	C	338	ARG	2.6
1	C	681	GLN	2.6
1	A	488	GLU	2.6
1	C	376	GLU	2.6
1	A	450	PRO	2.6
1	C	489	LYS	2.6
1	C	356	ASN	2.6
1	A	316	HIS	2.6
1	A	350	PHE	2.6
1	A	520	LEU	2.6
1	C	739	PRO	2.5
1	A	738	LEU	2.5
1	A	1028	LYS	2.5
1	C	345	GLU	2.5
1	C	363	GLN	2.5
1	A	322	ASN	2.5
1	A	333	ILE	2.5
1	A	330	GLN	2.5
1	A	712	ASP	2.4
1	A	531	PRO	2.4
1	A	342	LYS	2.4
1	A	981	LYS	2.4
1	A	474	GLU	2.4
1	A	363	GLN	2.4
1	A	662	LEU	2.4
1	C	419	ALA	2.4
1	A	405	LEU	2.3
1	C	768	PRO	2.3
1	C	678	VAL	2.3
1	A	320	LEU	2.3
1	A	528	LEU	2.3
1	C	961	LYS	2.3
1	A	532	PRO	2.3
1	A	963	ARG	2.3
1	C	774	GLU	2.3
1	C	490	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	449	LYS	2.3
1	C	371	LEU	2.3
1	A	1019	ALA	2.2
1	C	821	THR	2.2
1	A	609	PRO	2.2
1	C	954	GLY	2.2
1	A	736	ASP	2.2
1	C	384	PHE	2.2
1	A	327	LYS	2.2
1	A	776	VAL	2.2
1	C	492	LEU	2.2
1	C	884	GLY	2.2
1	A	419	ALA	2.2
1	A	332	ASN	2.2
1	A	336	ALA	2.2
1	A	961	LYS	2.2
1	A	515	GLU	2.1
1	C	939	GLU	2.1
2	B	26	MET	2.1
1	C	780	ILE	2.1
1	C	776	VAL	2.1
1	C	534	GLU	2.1
1	A	406	GLN	2.1
1	C	379	ARG	2.1
1	A	329	GLU	2.1
1	C	677	GLU	2.1
1	C	981	LYS	2.1
1	A	480	VAL	2.0
1	A	339	LEU	2.0
1	C	738	LEU	2.0
1	A	677	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

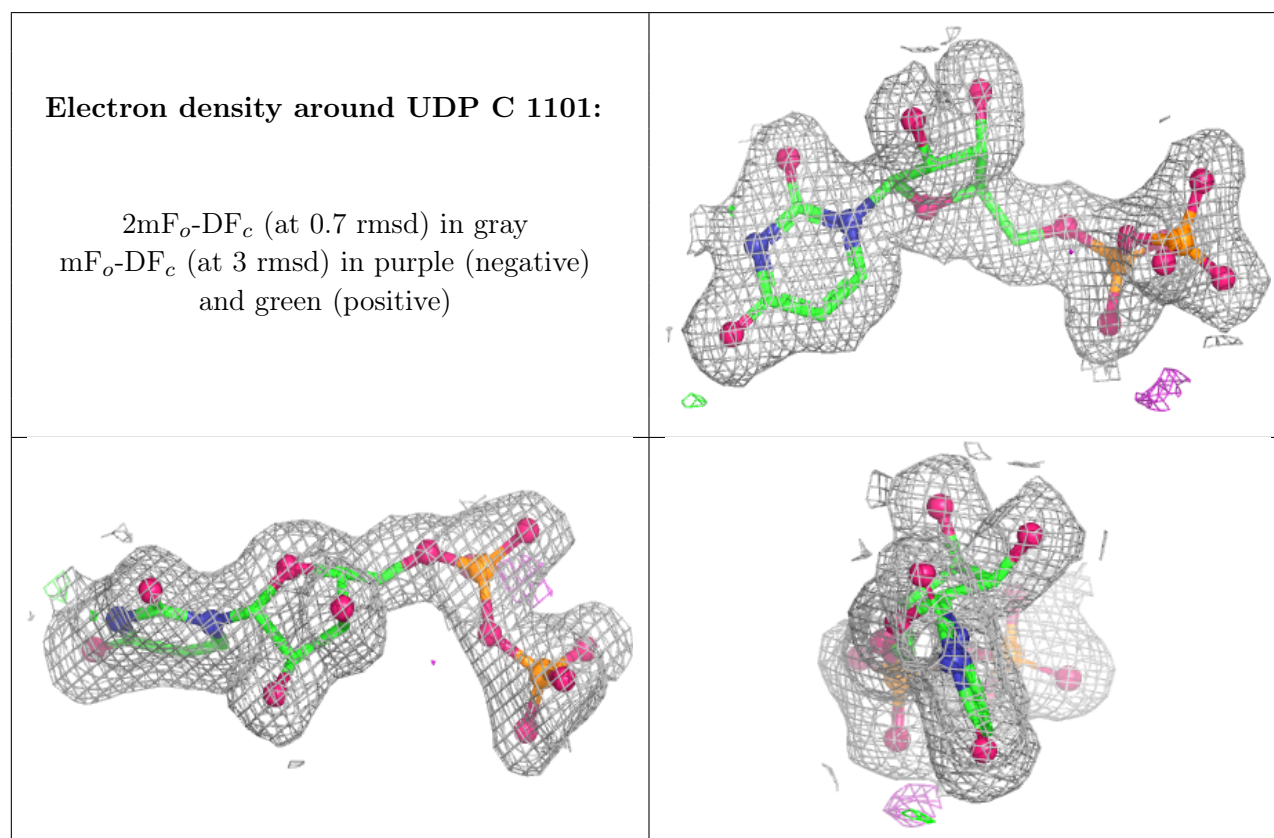
There are no oligosaccharides in this entry.

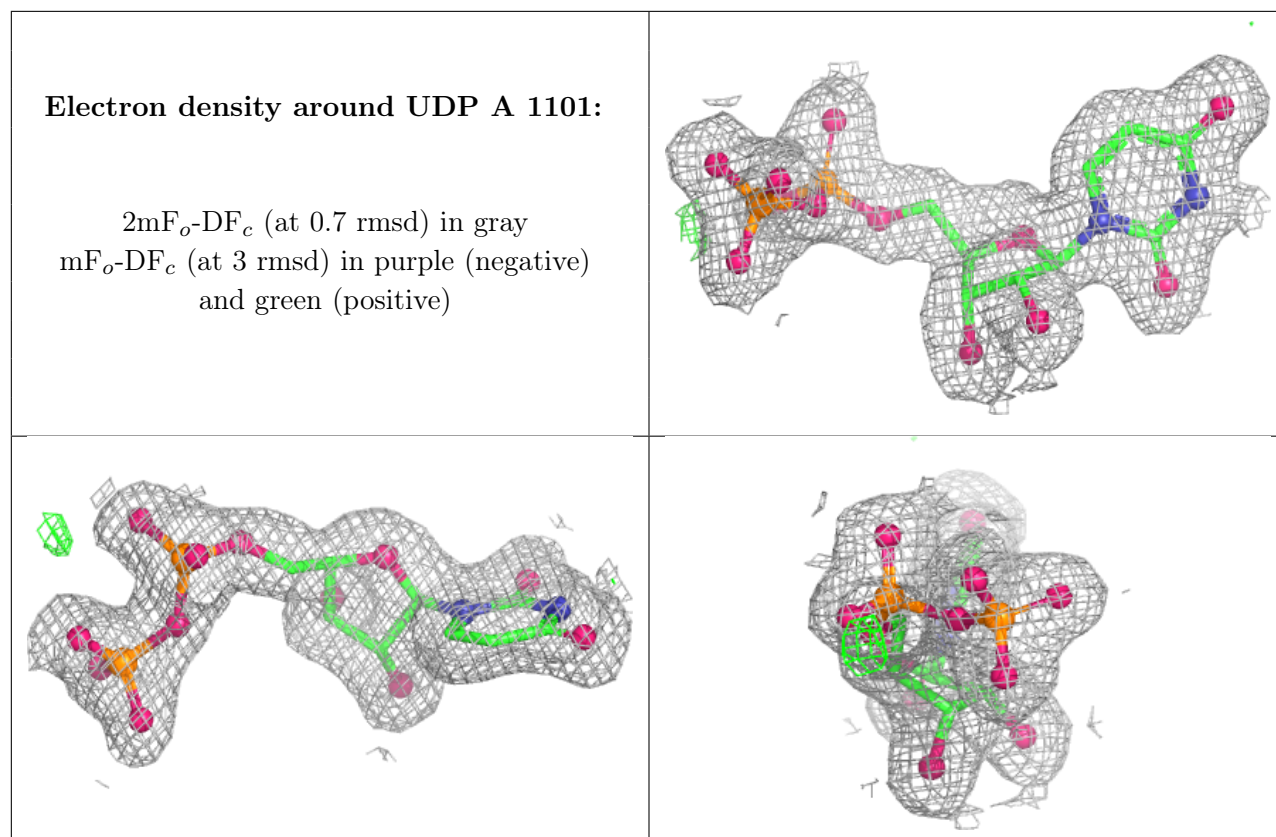
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	1102	5/5	0.80	0.17	66,66,66,67	0
5	0YT	B	101	14/15	0.93	0.09	14,20,29,31	0
5	0YT	D	101	14/15	0.93	0.09	14,19,28,31	0
4	SO4	D	102	5/5	0.94	0.13	41,43,45,47	0
4	SO4	B	102	5/5	0.96	0.11	41,42,45,45	0
3	UDP	C	1101	25/25	0.98	0.05	10,14,16,18	0
3	UDP	A	1101	25/25	0.98	0.05	10,13,16,17	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.