



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:01 PM UTC

PDB ID : 5HGV / pdb_00005hgv
Title : Structure of an O-GlcNAc transferase point mutant, D554N in complex with peptide
Authors : Janetzko, J.; Lazarus, M.B.; Walker, S.
Deposited on : 2016-01-08
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

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

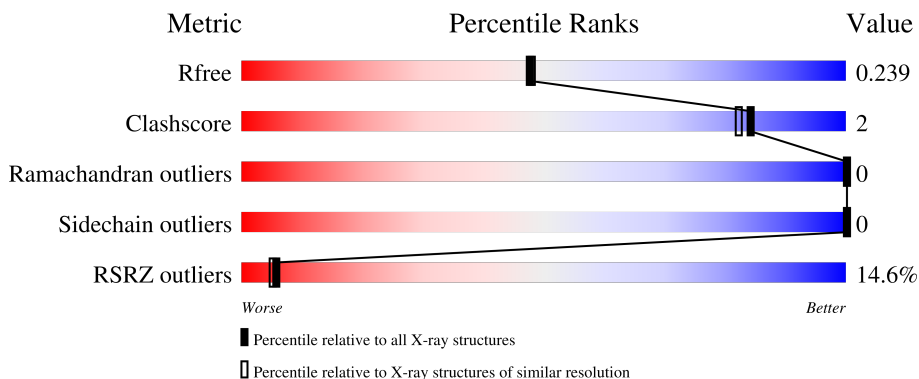
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 ≥ 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	719	13% 90% 6%
1	C	719	15% 88% 5% 6%
2	B	14	14% 79% 21%
2	D	14	7% 86% 14%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11958 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	8	0
			5536	3514	967	1018	37			
1	C	674	Total	C	N	O	S	0	7	0
			5367	3417	935	977	38			

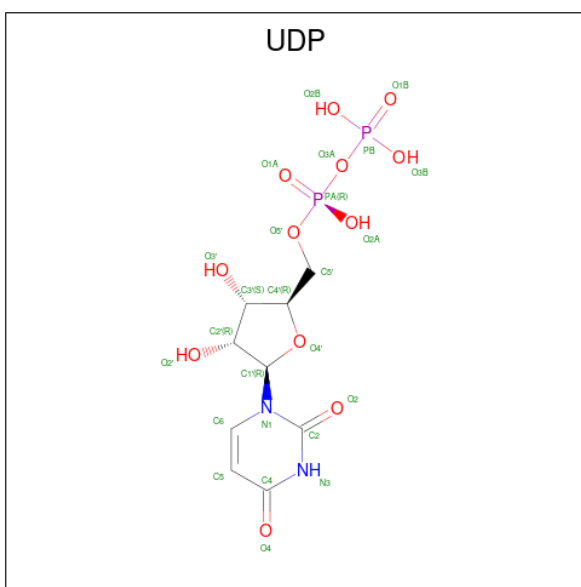
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	554	ASN	ASP	engineered mutation	UNP O15294
C	554	ASN	ASP	engineered mutation	UNP O15294

- Molecule 2 is a protein called TYR-PRO-GLY-GLY-SER-THR-PRO-VAL-SER-SER-ALA-ASN-MET-MET.

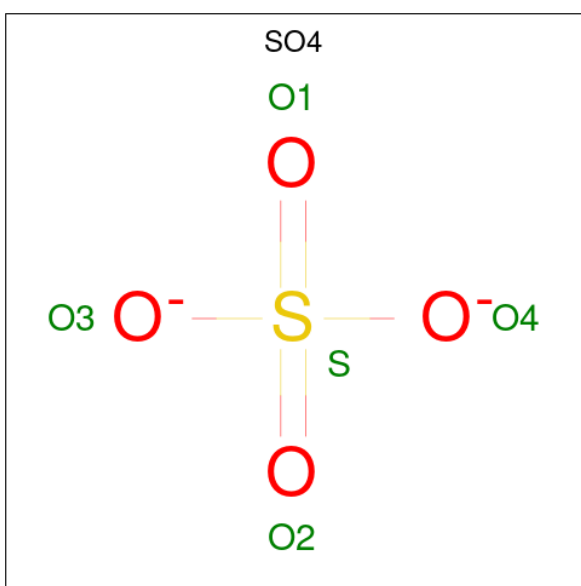
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	S	0	0	0
			95	58	15	20	2			
2	D	14	Total	C	N	O	S	0	0	0
			95	58	15	20	2			

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



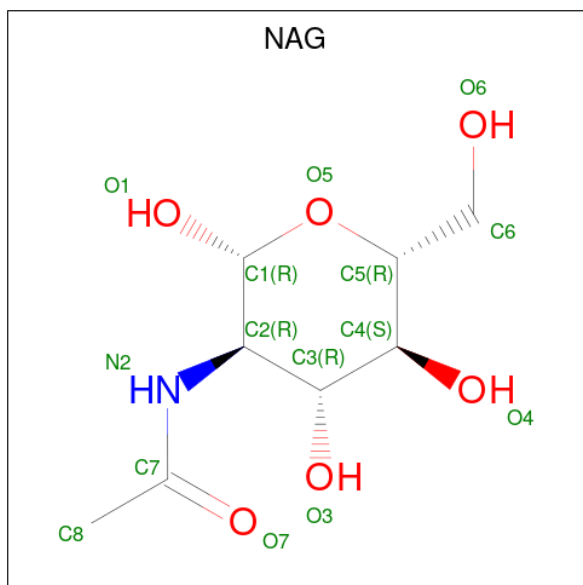
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

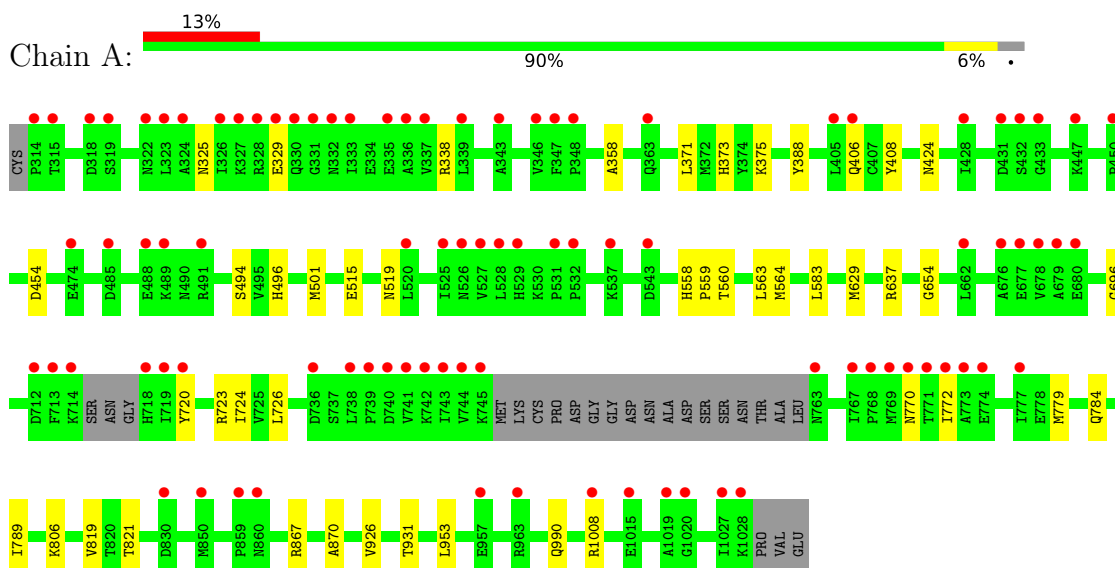
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	370	Total	O	0	0
			370	370		
6	B	14	Total	O	0	0
			14	14		
6	C	376	Total	O	0	0
			376	376		
6	D	12	Total	O	0	0
			12	12		

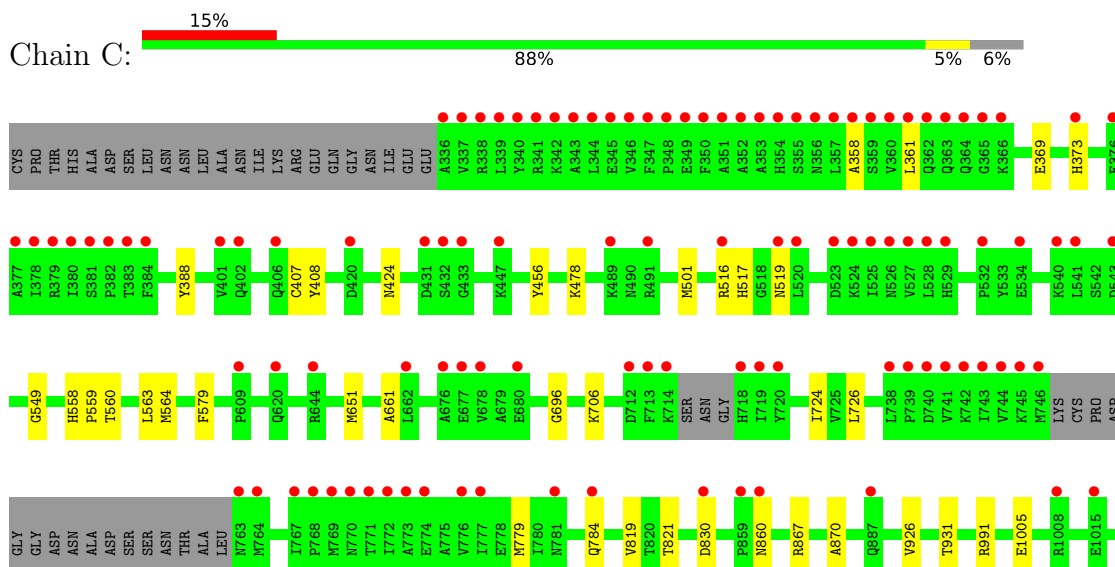
3 Residue-property plots

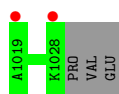
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

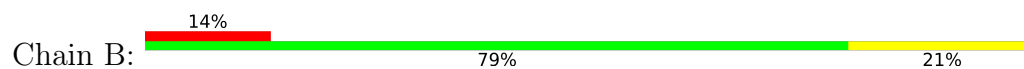


- Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit

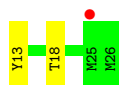
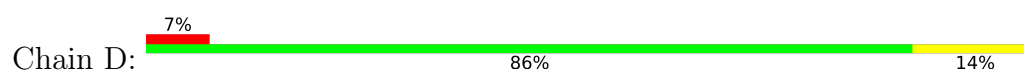




- Molecule 2: TYR-PRO-GLY-GLY-SER-THR-PRO-VAL-SER-SER-ALA-ASN-MET-MET



- Molecule 2: TYR-PRO-GLY-GLY-SER-THR-PRO-VAL-SER-SER-ALA-ASN-MET-MET



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.35Å 137.19Å 153.07Å 90.00° 103.05° 90.00°	Depositor
Resolution (Å)	40.92 – 2.05 40.92 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.0 (40.92-2.05) 95.0 (40.92-2.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.05Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.217 , 0.237 0.218 , 0.239	Depositor DCC
R_{free} test set	5894 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.4	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	0.93	EDS
Total number of atoms	11958	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.63% 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: NAG, 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	0.18	0/5688	0.37	0/7713
1	C	0.19	0/5515	0.37	0/7478
2	B	0.25	0/97	0.42	0/131
2	D	0.26	0/97	0.48	0/131
All	All	0.19	0/11397	0.37	0/15453

There are no bond length outliers.

There are no bond angle outliers.

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	5536	0	5522	27	0
1	C	5367	0	5365	22	0
2	B	95	0	87	2	0
2	D	95	0	87	1	0
3	A	25	0	11	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	14	0	13	1	0
5	D	14	0	13	1	0
6	A	370	0	0	6	0
6	B	14	0	0	0	0
6	C	376	0	0	3	0
6	D	12	0	0	0	0
All	All	11958	0	11109	51	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 (51) 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:661:ALA:O	6:C:1202:HOH:O	2.05	0.75
1:C:517:HIS:NE2	6:C:1201:HOH:O	1.97	0.64
1:C:516:ARG:NH2	1:C:519:ASN:OD1	2.31	0.62
1:A:338:ARG:O	6:A:1202:HOH:O	2.16	0.61
2:D:13:TYR:N	2:D:18:THR:HG1	1.99	0.60
1:A:1008:ARG:NH2	6:A:1210:HOH:O	2.36	0.58
2:B:13:TYR:N	2:B:18:THR:HG1	2.02	0.57
1:C:358:ALA:HB2	1:C:373:HIS:HB2	1.87	0.56
1:A:371:LEU:HG	1:A:375:LYS:HE3	1.88	0.55
1:C:361:LEU:HD13	1:C:369:GLU:HB3	1.89	0.55
1:C:1005:GLU:HG3	6:C:1474:HOH:O	2.07	0.55
1:A:770:ASN:ND2	6:A:1211:HOH:O	2.38	0.52
1:A:358:ALA:HB2	1:A:373:HIS:HB2	1.92	0.52
1:A:953:LEU:O	1:A:990[B]:GLN:NE2	2.44	0.50
1:C:867:ARG:HB3	1:C:870:ALA:HA	1.92	0.50
1:A:779:MET:HG3	1:A:784:GLN:HB2	1.94	0.49
1:A:806:LYS:NZ	6:A:1205:HOH:O	2.26	0.49
1:C:926:VAL:HG22	1:C:931:THR:HB	1.95	0.48
1:A:926:VAL:HG22	1:A:931:THR:HB	1.96	0.48
1:C:501:MET:HE1	5:D:101:NAG:H81	1.96	0.48
1:A:325:ASN:O	1:A:329:GLU:HG2	2.15	0.46
1:A:408:TYR:CZ	1:A:424:ASN:HB3	2.51	0.46
1:A:867:ARG:HB3	1:A:870:ALA:HA	1.97	0.45
1:C:724:ILE:HG23	1:C:821:THR:HG22	1.99	0.45
1:A:558:HIS:CG	1:A:559:PRO:HD2	2.52	0.44
1:C:456:TYR:CZ	1:C:478:LYS:HD3	2.52	0.44
1:C:706:LYS:O	1:C:991:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:830:ASP:O	1:C:860:ASN:ND2	2.50	0.44
1:C:408:TYR:CZ	1:C:424:ASN:HB3	2.53	0.44
1:C:726[A]:LEU:CD2	1:C:819:VAL:HG22	2.48	0.43
1:A:406:GLN:OE1	6:A:1204:HOH:O	2.21	0.43
1:A:563:LEU:HA	1:A:696:GLY:HA2	2.00	0.43
1:A:454:ASP:OD1	1:A:494:SER:OG	2.35	0.42
1:C:560:THR:O	1:C:564:MET:HG3	2.19	0.42
1:C:558:HIS:CG	1:C:559:PRO:HD2	2.55	0.42
1:C:779:MET:HG3	1:C:784:GLN:HB2	2.01	0.42
1:A:724:ILE:HG23	1:A:821:THR:HG22	2.01	0.42
1:A:496:HIS:CE1	2:B:23:ALA:HB1	2.55	0.42
1:A:560:THR:O	1:A:564:MET:HG3	2.20	0.42
1:A:501:MET:HE1	5:B:101:NAG:H81	2.03	0.41
1:A:720:TYR:HB3	1:A:723:ARG:HD3	2.03	0.41
1:C:549:GLY:HA2	1:C:579:PHE:O	2.20	0.41
1:A:388:TYR:OH	6:A:1201:HOH:O	2.10	0.41
1:A:515[A]:GLU:OE2	1:A:519:ASN:ND2	2.53	0.41
1:A:583:LEU:HD22	1:A:637:ARG:HD3	2.03	0.41
1:C:651:MET:HE3	1:C:651:MET:HB3	1.95	0.41
1:C:388:TYR:O	1:C:407:CYS:HB3	2.21	0.40
1:A:629:MET:O	1:A:654:GLY:HA3	2.22	0.40
1:A:726:LEU:CD2	1:A:819:VAL:HG22	2.52	0.40
1:A:772:ILE:HG23	1:A:789:ILE:HD13	2.02	0.40
1:C:563:LEU:HA	1:C:696:GLY:HA2	2.03	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	698/719 (97%)	687 (98%)	11 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	675/719 (94%)	664 (98%)	11 (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	1397/1466 (95%)	1375 (98%)	22 (2%)	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	606/616 (98%)	606 (100%)	0	100	100
1	C	586/616 (95%)	586 (100%)	0	100	100
2	B	11/11 (100%)	11 (100%)	0	100	100
2	D	11/11 (100%)	11 (100%)	0	100	100
All	All	1214/1254 (97%)	1214 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	GLN
1	A	727	ASN
1	A	763	ASN
1	A	802	GLN
1	A	906	GLN
1	C	802	GLN
1	C	805	ASN
1	C	849	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	0.24	0	6,6,6	0.25	0
4	SO4	B	102	-	4,4,4	0.22	0	6,6,6	0.15	0
4	SO4	A	1102	-	4,4,4	0.28	0	6,6,6	0.12	0
3	UDP	A	1101	-	25,26,26	1.01	2 (8%)	38,40,40	1.59	5 (13%)
5	NAG	D	101	2	14,14,15	1.02	1 (7%)	17,19,21	0.64	1 (5%)
3	UDP	C	1101	-	25,26,26	1.02	2 (8%)	38,40,40	1.59	5 (13%)
5	NAG	B	101	2	14,14,15	0.86	1 (7%)	17,19,21	0.65	1 (5%)

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	NAG	D	101	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	C	1101	-	-	4/16/32/32	0/2/2/2
5	NAG	B	101	2	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	101	NAG	C1-C2	3.37	1.56	1.52
5	B	101	NAG	C1-C2	2.91	1.56	1.52
3	C	1101	UDP	PA-O3A	2.35	1.62	1.59
3	A	1101	UDP	PA-O3A	2.18	1.61	1.59
3	A	1101	UDP	C6-C5	2.07	1.39	1.35
3	C	1101	UDP	C6-C5	2.01	1.39	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	UDP	C4-N3-C2	-5.69	119.55	126.61
3	C	1101	UDP	C4-N3-C2	-5.67	119.58	126.61
3	A	1101	UDP	N3-C2-N1	4.80	121.14	114.89
3	C	1101	UDP	N3-C2-N1	4.29	120.48	114.89
3	C	1101	UDP	C5-C4-N3	3.69	119.97	114.80
3	A	1101	UDP	C5-C4-N3	3.37	119.53	114.80
3	C	1101	UDP	O4-C4-C5	-2.97	120.04	125.16
3	C	1101	UDP	O2-C2-N1	-2.52	119.51	122.80
3	A	1101	UDP	O2-C2-N1	-2.45	119.60	122.80
3	A	1101	UDP	O4-C4-C5	-2.27	121.25	125.16
5	B	101	NAG	C1-O5-C5	2.21	115.14	112.19
5	D	101	NAG	C1-O5-C5	2.08	114.97	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

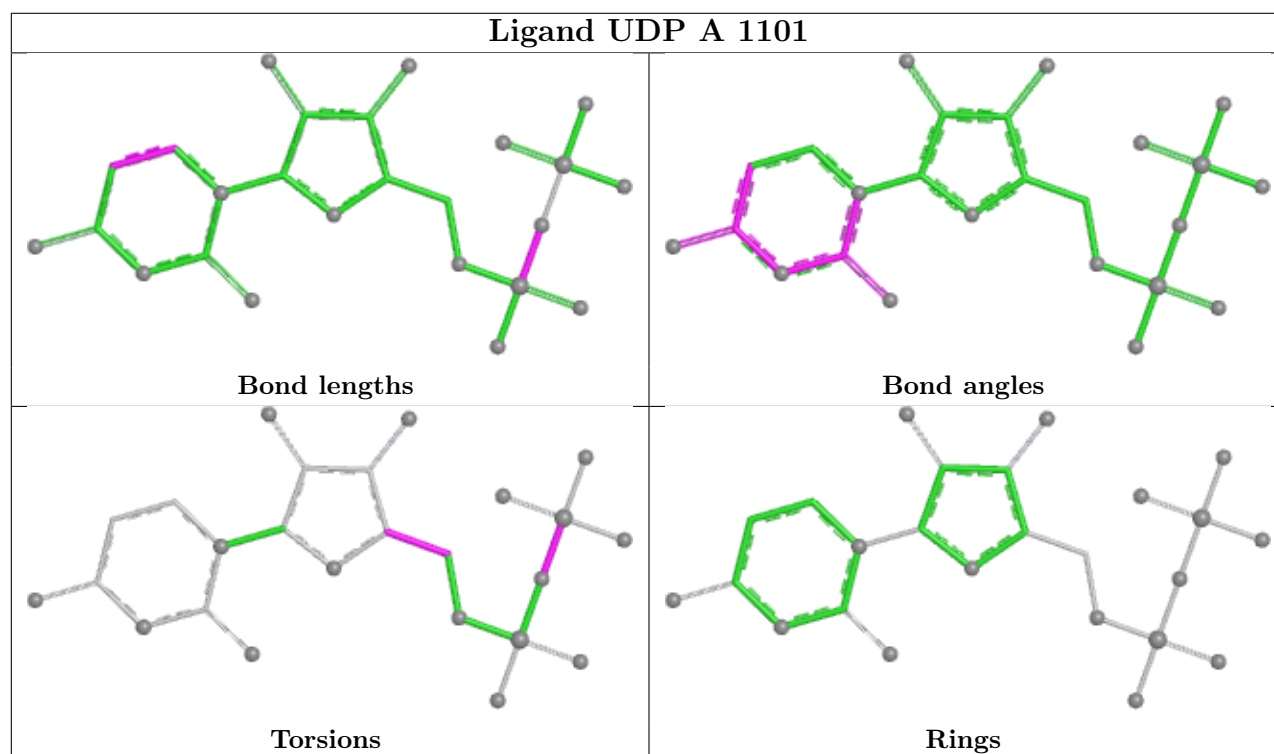
Mol	Chain	Res	Type	Atoms
3	C	1101	UDP	PA-O3A-PB-O3B
3	A	1101	UDP	O4'-C4'-C5'-O5'
3	C	1101	UDP	O4'-C4'-C5'-O5'
3	A	1101	UDP	C3'-C4'-C5'-O5'
3	C	1101	UDP	C3'-C4'-C5'-O5'
3	A	1101	UDP	PA-O3A-PB-O3B
3	C	1101	UDP	C5'-O5'-PA-O1A

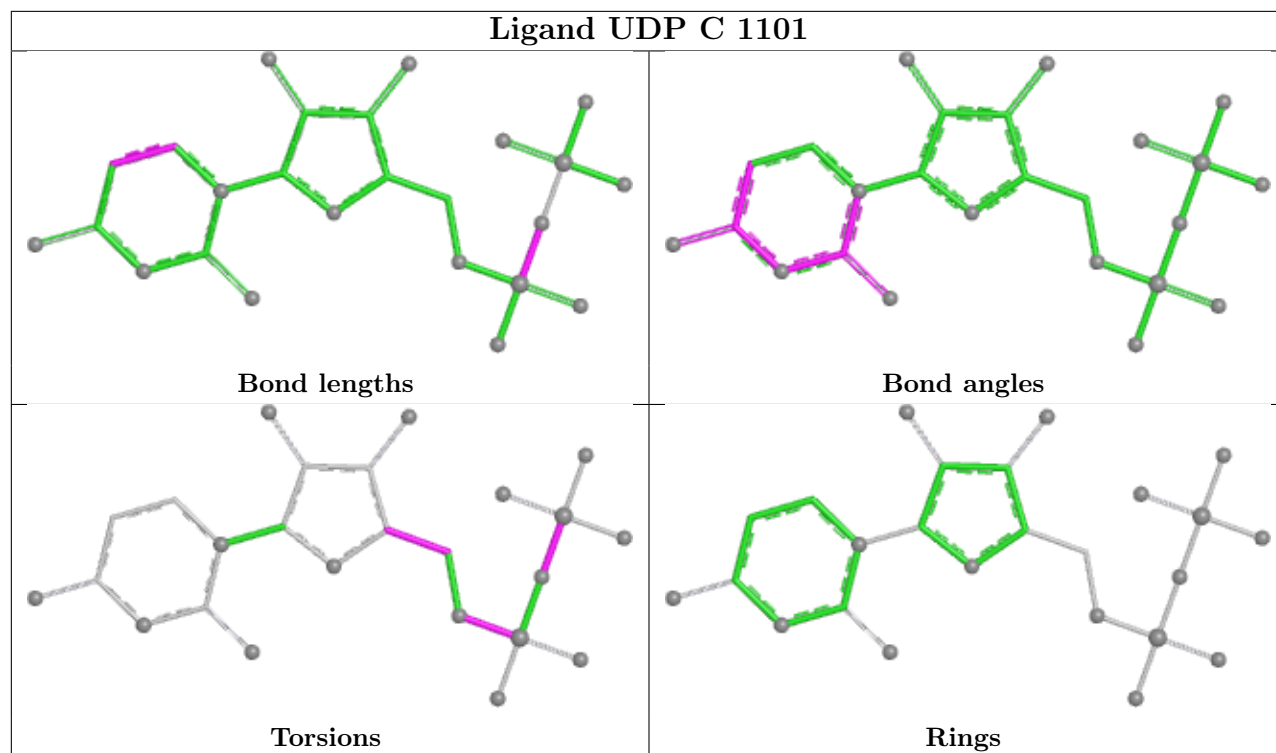
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	101	NAG	1	0
5	B	101	NAG	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, 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	695/719 (96%)	0.70	90 (12%) 7 7	12, 28, 59, 87	8 (1%)
1	C	674/719 (93%)	0.78	111 (16%) 4 4	12, 27, 60, 87	7 (1%)
2	B	14/14 (100%)	0.41	2 (14%) 6 5	17, 25, 54, 54	0
2	D	14/14 (100%)	0.27	1 (7%) 22 22	16, 26, 51, 52	0
All	All	1397/1466 (95%)	0.73	204 (14%) 6 5	12, 28, 59, 87	15 (1%)

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	714	LYS	7.2
1	A	772	ILE	7.0
1	A	769	MET	6.8
1	C	360	VAL	6.8
1	C	718	HIS	6.5
1	C	713	PHE	6.5
1	A	740	ASP	6.4
1	A	745	LYS	6.3
1	A	314	PRO	6.2
1	C	746	MET	6.1
1	C	772	ILE	6.1
1	C	336	ALA	6.0
1	C	860	ASN	5.6
1	A	860	ASN	5.5
1	A	718	HIS	5.5
1	C	714	LYS	5.5
1	C	347	PHE	5.5
1	A	326	ILE	5.4
1	A	713	PHE	5.3
1	C	350	PHE	5.3
1	A	330	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	337	VAL	5.1
1	C	346	VAL	5.0
1	A	770	ASN	5.0
1	A	763	ASN	5.0
1	C	348	PRO	4.9
1	C	745	LYS	4.9
1	C	339	LEU	4.6
1	C	769	MET	4.6
1	C	719	ILE	4.6
1	C	351	ALA	4.6
1	C	777	ILE	4.6
1	C	770	ASN	4.5
1	C	431	ASP	4.5
1	C	680	GLU	4.5
1	C	771	THR	4.4
1	C	720	TYR	4.4
1	A	328	ARG	4.4
1	C	526	ASN	4.4
1	C	773	ALA	4.4
1	C	344	LEU	4.3
1	C	740	ASP	4.3
1	A	742	LYS	4.3
1	C	830	ASP	4.3
1	C	383	THR	4.2
1	A	744	VAL	4.1
1	C	353	ALA	4.0
1	A	767	ILE	4.0
1	A	720	TYR	3.9
1	A	485	ASP	3.7
1	A	678	VAL	3.7
1	C	527	VAL	3.7
1	A	491	ARG	3.7
1	C	356	ASN	3.7
1	C	528	LEU	3.7
1	C	354	HIS	3.7
1	C	358	ALA	3.7
1	C	361	LEU	3.6
1	C	380	ILE	3.6
1	A	526	ASN	3.6
1	A	680	GLU	3.6
1	A	830	ASP	3.5
1	C	359	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	381	SER	3.5
1	C	741	VAL	3.5
1	C	343	ALA	3.5
1	A	433	GLY	3.4
1	A	323	LEU	3.4
1	A	333	ILE	3.4
1	A	739	PRO	3.4
1	A	768	PRO	3.4
1	C	364	GLN	3.4
1	A	771	THR	3.4
1	A	319[A]	SER	3.4
1	C	355	SER	3.3
2	B	25	MET	3.3
1	A	431	ASP	3.3
1	A	774	GLU	3.3
1	A	743	ILE	3.2
1	A	331	GLY	3.2
1	C	768	PRO	3.2
1	C	744	VAL	3.2
1	C	525	ILE	3.2
1	A	543	ASP	3.2
1	C	774	GLU	3.2
1	A	346	VAL	3.1
1	A	520	LEU	3.1
1	C	357	LEU	3.1
1	A	363	GLN	3.1
1	C	516	ARG	3.1
1	C	338	ARG	3.1
1	A	777	ILE	3.1
1	C	340	TYR	3.1
1	A	677	GLU	3.1
1	C	523	ASP	3.1
1	C	541	LEU	3.1
1	C	384	PHE	3.0
1	C	742	LYS	3.0
1	C	781	ASN	3.0
1	A	488	GLU	3.0
1	C	376	GLU	3.0
1	C	712	ASP	3.0
1	A	676	ALA	3.0
1	A	1019	ALA	3.0
1	C	352	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	401	VAL	3.0
1	C	1015	GLU	3.0
1	A	719	ILE	3.0
1	A	336	ALA	2.9
1	A	339	LEU	2.9
2	D	25	MET	2.9
1	C	1028	LYS	2.9
1	C	373	HIS	2.9
1	A	712	ASP	2.8
1	A	773	ALA	2.8
1	A	347	PHE	2.8
1	C	433	GLY	2.8
1	A	337	VAL	2.8
1	A	447	LYS	2.8
1	C	524	LYS	2.8
1	C	763	ASN	2.8
1	A	335	GLU	2.8
1	A	662	LEU	2.8
1	A	741	VAL	2.8
1	C	529	HIS	2.7
1	C	365	GLY	2.7
1	C	382	PRO	2.7
1	C	342	LYS	2.7
1	C	491	ARG	2.7
1	A	527	VAL	2.6
1	C	363	GLN	2.6
1	A	529	HIS	2.6
1	C	676	ALA	2.6
1	C	1019	ALA	2.6
1	A	318	ASP	2.6
1	C	420	ASP	2.6
1	A	432	SER	2.6
1	C	406	GLN	2.6
1	C	743	ILE	2.6
1	C	887	GLN	2.6
1	A	859	PRO	2.6
1	A	474	GLU	2.5
1	C	377	ALA	2.5
1	C	609	PRO	2.5
1	A	528	LEU	2.5
1	A	537	LYS	2.5
1	C	644	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	519	ASN	2.5
1	C	1008	ARG	2.5
1	C	776	VAL	2.4
1	C	366	LYS	2.4
1	C	678	VAL	2.4
1	C	489	LYS	2.4
1	A	679	ALA	2.4
1	A	428	ILE	2.4
1	C	859	PRO	2.4
1	A	489	LYS	2.3
1	C	447	LYS	2.3
1	C	532	PRO	2.3
1	C	620	GLN	2.3
1	A	738	LEU	2.3
1	C	662	LEU	2.3
1	A	963	ARG	2.3
1	C	349	GLU	2.3
1	A	322	ASN	2.3
1	A	332	ASN	2.3
1	A	324	ALA	2.3
1	C	379	ARG	2.3
1	A	1028	LYS	2.3
1	C	764	MET	2.3
1	A	315	THR	2.3
1	C	739	PRO	2.3
1	C	520	LEU	2.3
1	A	1015	GLU	2.2
1	C	402	GLN	2.2
1	A	1027	ILE	2.2
1	A	327	LYS	2.2
1	A	450	PRO	2.2
1	A	531	PRO	2.2
2	B	26	MET	2.2
1	A	1020	GLY	2.2
1	C	345	GLU	2.2
1	A	406	GLN	2.2
1	A	532	PRO	2.2
1	A	957	GLU	2.2
1	C	677	GLU	2.2
1	C	784	GLN	2.2
1	A	736	ASP	2.2
1	A	405	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	738	LEU	2.1
1	C	378	ILE	2.1
1	A	329	GLU	2.1
1	C	543	ASP	2.1
1	A	525	ILE	2.1
1	A	1008	ARG	2.1
1	C	432	SER	2.1
1	C	534	GLU	2.1
1	C	362	GLN	2.1
1	A	343	ALA	2.1
1	C	540	LYS	2.0
1	C	767	ILE	2.0
1	A	850[A]	MET	2.0
1	C	341	ARG	2.0
1	A	348	PRO	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](#)

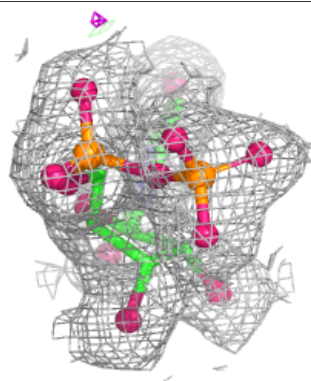
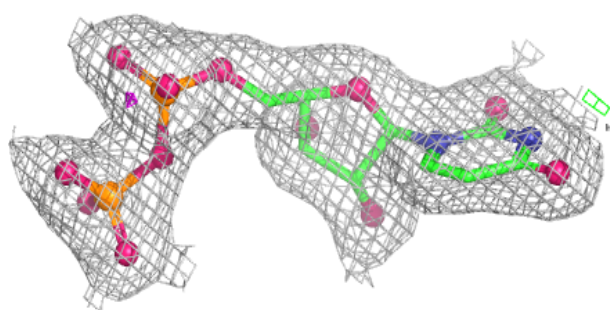
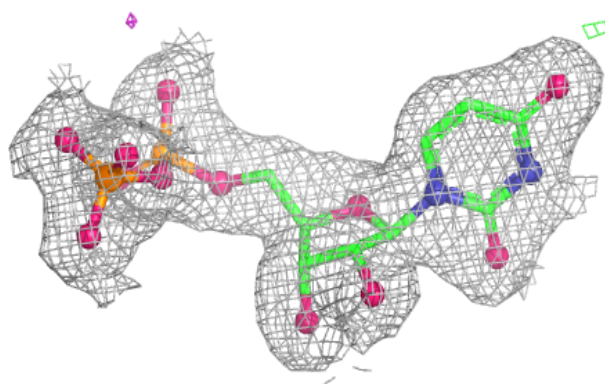
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

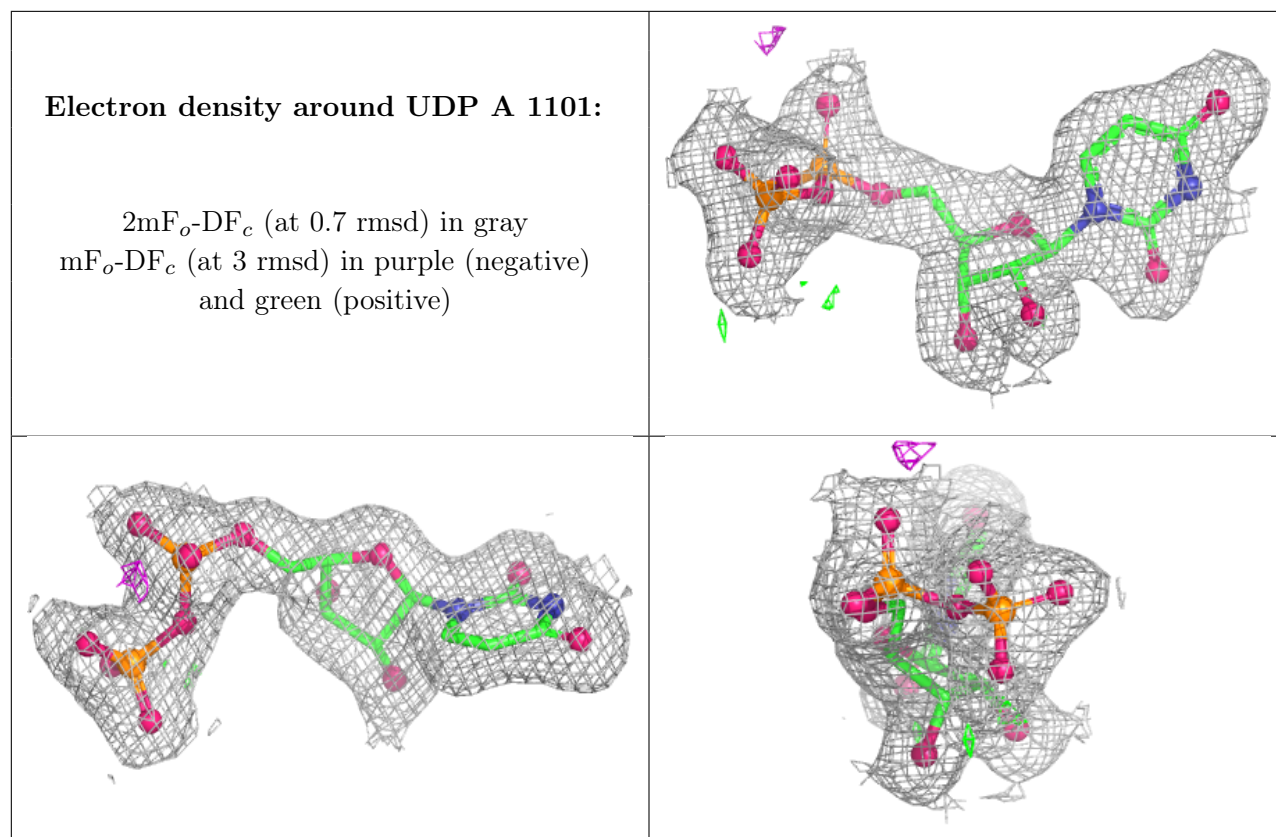
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	1102	5/5	0.74	0.20	78,78,79,79	0
5	NAG	B	101	14/15	0.93	0.07	15,17,18,19	0
4	SO4	D	102	5/5	0.94	0.12	39,40,42,42	0
5	NAG	D	101	14/15	0.94	0.07	13,15,17,18	0
4	SO4	B	102	5/5	0.96	0.10	40,41,42,43	0
3	UDP	C	1101	25/25	0.98	0.05	11,15,17,18	0
3	UDP	A	1101	25/25	0.98	0.05	10,14,17,19	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 UDP C 1101:

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.