Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 10:59 PM EDT

PDB ID	:	4GZ3
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 (i) 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 (i)) were used in the production of this report:

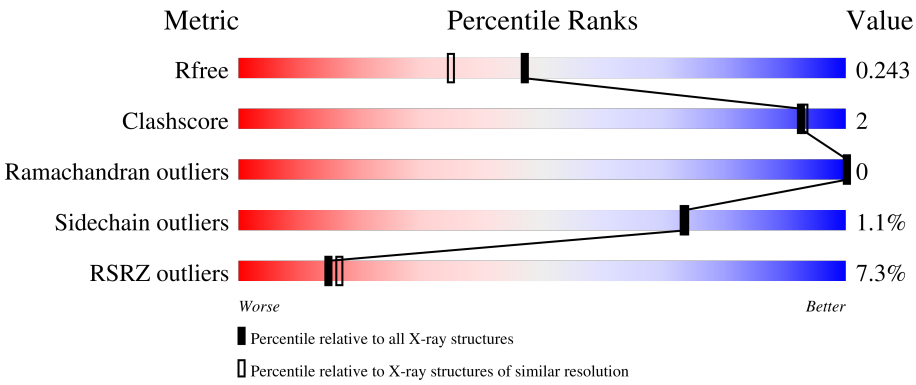
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 <=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	8% 93%
1	C	723	6% 88% 5% 7%
2	B	14	64% 36%
2	D	14	86% 14%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	695	5530	3510	966	1017	37	0	7	0
1	C	674	5361	3413	934	976	38	0	6	0

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

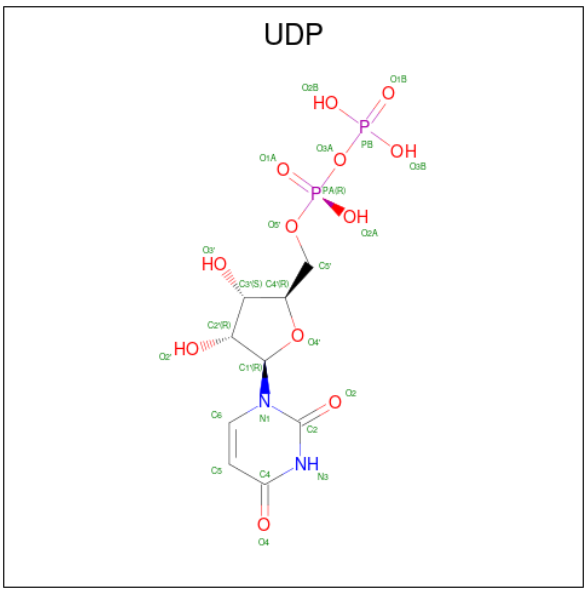
- Molecule 2 is a protein called Casein kinase II subunit alpha.

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

There are 2 discrepancies between the modelled and reference sequences:

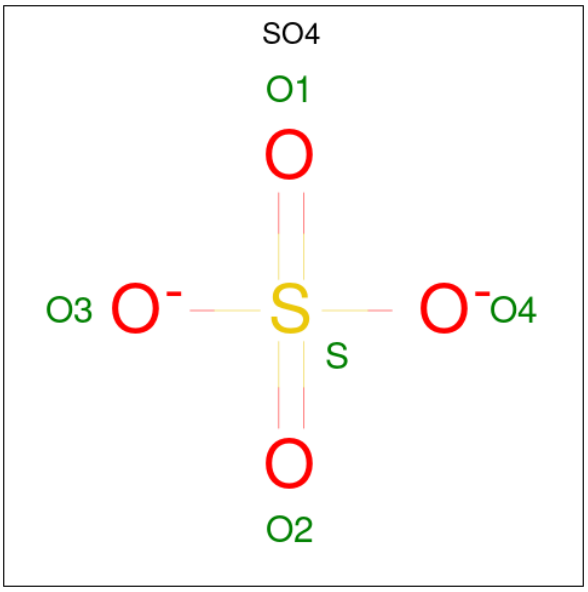
Chain	Residue	Modelled	Actual	Comment	Reference
B	13	TYR	-	expression tag	UNP P68400
D	13	TYR	-	expression tag	UNP P68400

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



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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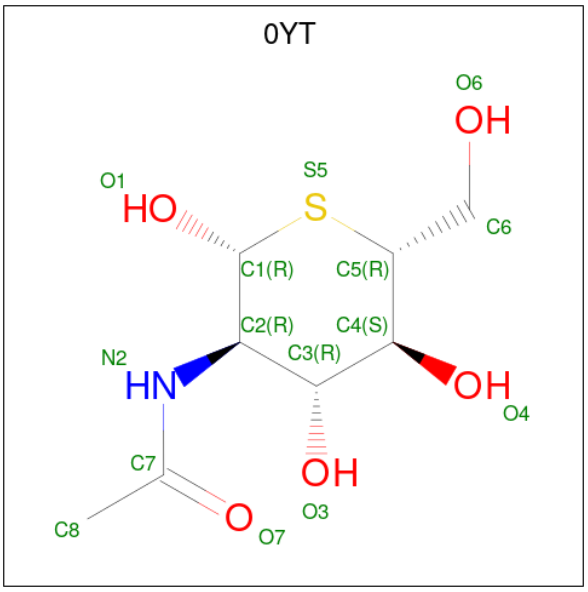
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
4	B	1	5	4	1		0	0
			Total	O	S			
4	D	1	5	4	1		0	0

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



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

- Molecule 6 is water.

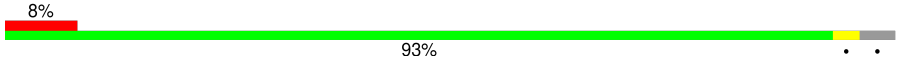
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	419	419	419	0	0
			Total	O		
6	B	8	8	8	0	0
			Total	O		
6	C	397	397	397	0	0
			Total	O		
6	D	12	12	12	0	0

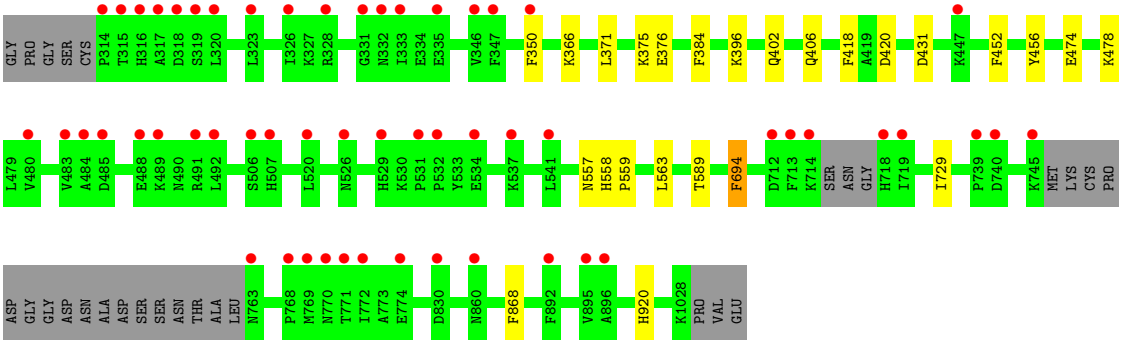
3 Residue-property plots (i)

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

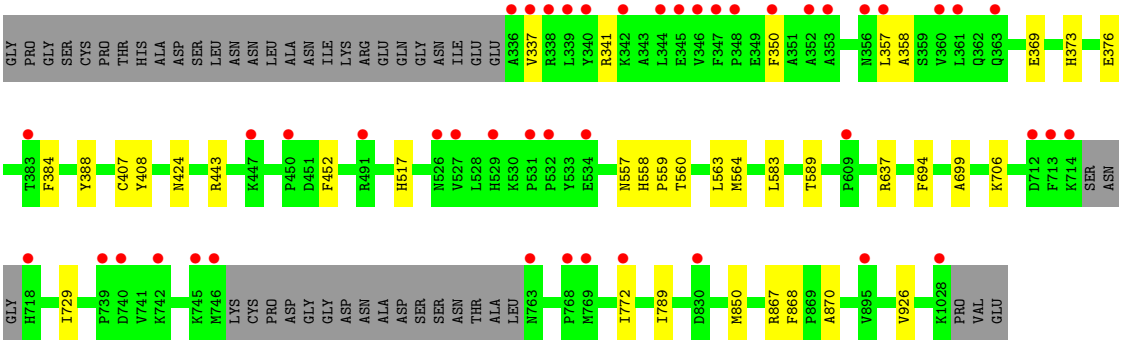
Chain A:





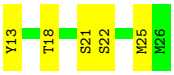
• Molecule 1: UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit

Chain C:



• Molecule 2: Casein kinase II subunit alpha

Chain B:



• Molecule 2: Casein kinase II subunit alpha

Chain D:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.03%)	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 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, 0YT, 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	0.28	0/5679	0.46	0/7701
1	C	0.28	0/5506	0.45	0/7466
2	B	0.30	0/97	0.45	0/131
2	D	0.28	0/97	0.45	0/131
All	All	0.28	0/11379	0.46	0/15429

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	5530	0	5514	13	0
1	C	5361	0	5357	18	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	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	34	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 (34) 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
2:B:13:TYR:N	2:B:18:THR:HG1	1.95	0.65
1:C:517:HIS:NE2	6:C:1533:HOH:O	2.30	0.64
2:D:13:TYR:N	2:D:18:THR:HG1	1.98	0.60
1:A:376:GLU:HG2	6:A:1421:HOH:O	2.05	0.55
1:A:396:LYS:NZ	1:A:431:ASP:OD2	2.38	0.55
1:C:376:GLU:HG2	6:C:1351:HOH:O	2.08	0.54
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:A:366:LYS:NZ	6:A:1411:HOH:O	2.38	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
2:B:21:SER:HA	6:B:204:HOH:O	2.20	0.42
1:C:850[B]:MET:HE2	1:C:850[B]:MET:HB2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:560:THR:O	1:C:564:MET:HG3	2.22	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	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 (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	605/618 (98%)	600 (99%)	5 (1%)	81	82
1	C	585/618 (95%)	579 (99%)	6 (1%)	76	76
2	B	11/11 (100%)	9 (82%)	2 (18%)	1	0
2	D	11/11 (100%)	11 (100%)	0	100	100
All	All	1212/1258 (96%)	1199 (99%)	13 (1%)	73	73

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	350	PHE
1	A	384	PHE
1	A	452	PHE
1	A	694	PHE
1	A	868	PHE
2	B	22	SER
2	B	25	MET
1	C	350	PHE
1	C	384	PHE
1	C	452	PHE
1	C	694	PHE
1	C	868	PHE
1	C	926	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	$\#\|Z\| > 2$
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%)
4	SO4	D	102	-	4,4,4	0.26	0	6,6,6	0.18	0
5	0YT	B	101	2	12,14,15	1.30	1 (8%)	12,19,21	1.34	2 (16%)
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%)

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

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(^{o})	Ideal(^{o})
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.

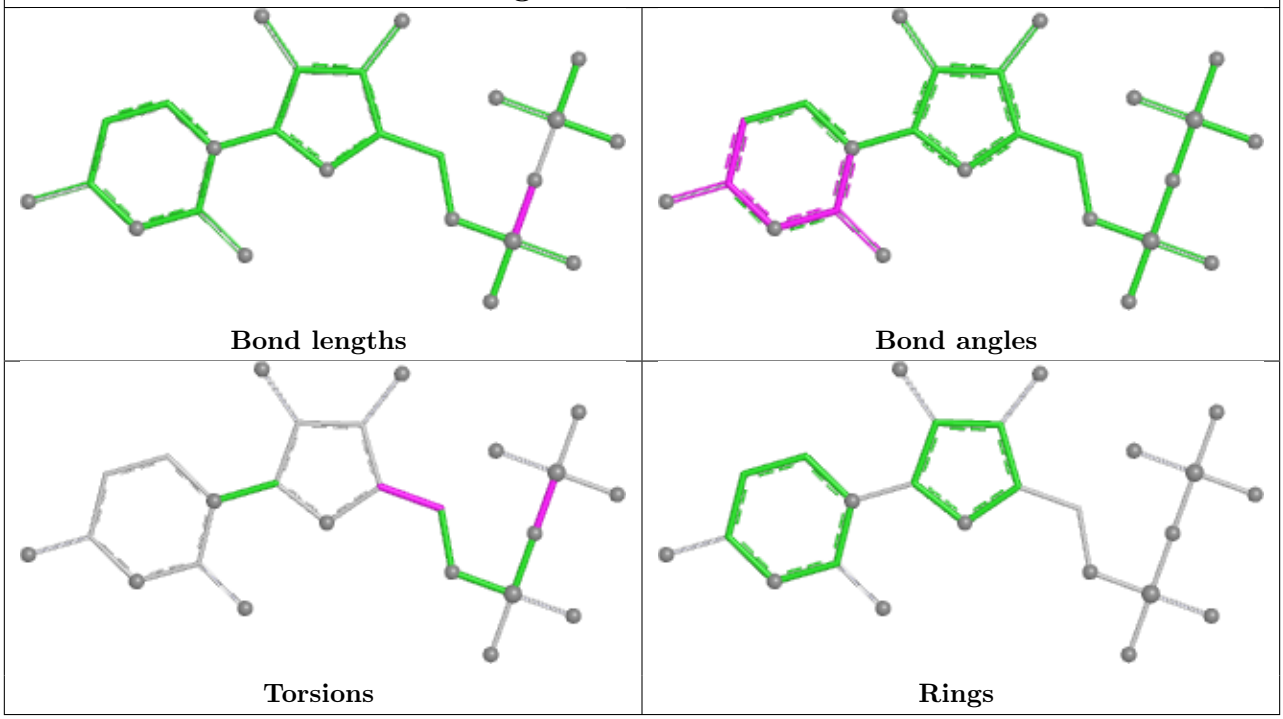
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	101	0YT	1	0
5	B	101	0YT	1	0

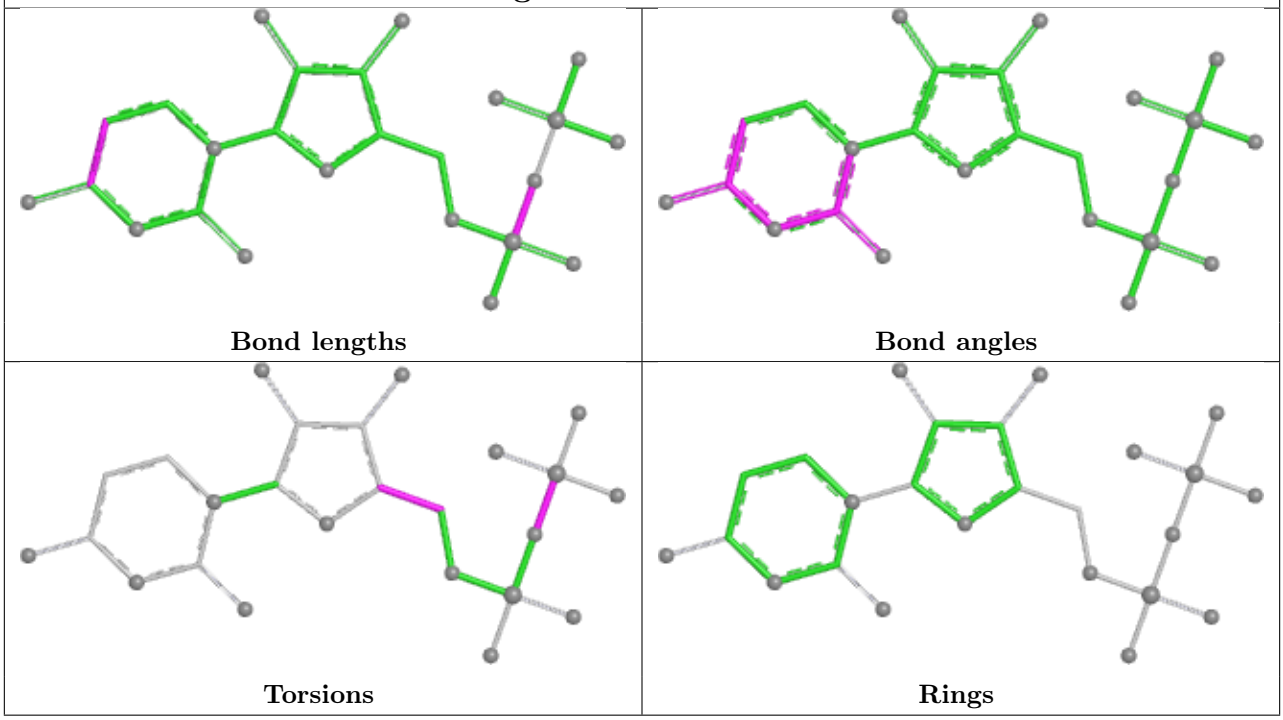
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand UDP A 1101



Ligand UDP C 1101



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.37	56 (8%) 12 13	13, 25, 55, 92	0
1	C	674/723 (93%)	0.38	46 (6%) 17 19	13, 24, 54, 95	0
2	B	14/14 (100%)	0.20	0 100 100	15, 23, 58, 58	0
2	D	14/14 (100%)	0.16	0 100 100	16, 24, 54, 55	0
All	All	1397/1474 (94%)	0.37	102 (7%) 15 16	13, 24, 55, 95	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	718	HIS	8.4
1	C	339	LEU	7.3
1	A	718	HIS	6.6
1	A	769	MET	6.6
1	C	347	PHE	6.5
1	A	713	PHE	6.1
1	C	338	ARG	5.9
1	C	346	VAL	5.8
1	A	491	ARG	5.4
1	A	314	PRO	5.3
1	C	769	MET	5.3
1	C	337	VAL	5.2
1	C	350	PHE	5.1
1	A	315	THR	5.1
1	A	740	ASP	5.0
1	A	331	GLY	5.0
1	A	772	ILE	4.9
1	A	714	LYS	4.6
1	C	348	PRO	4.6
1	C	713	PHE	4.4
1	C	344	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	342	LYS	4.4
1	A	526	ASN	4.3
1	C	526	ASN	4.2
1	C	746	MET	4.1
1	A	507	HIS	4.0
1	A	316	HIS	4.0
1	C	740	ASP	4.0
1	C	340	TYR	4.0
1	A	323	LEU	4.0
1	A	532	PRO	3.8
1	A	347	PHE	3.8
1	A	326	ILE	3.6
1	A	745	LYS	3.5
1	A	492	LEU	3.5
1	C	714	LYS	3.5
1	A	319[A]	SER	3.5
1	A	529	HIS	3.4
1	C	529	HIS	3.4
1	C	532	PRO	3.4
1	C	768	PRO	3.4
1	C	745	LYS	3.3
1	C	363	GLN	3.3
1	C	357	LEU	3.3
1	C	534	GLU	3.3
1	A	534	GLU	3.2
1	C	352	ALA	3.1
1	C	712	ASP	3.1
1	A	763	ASN	3.0
1	A	768	PRO	3.0
1	C	772	ILE	3.0
1	A	317	ALA	3.0
1	A	447	LYS	3.0
1	C	383	THR	3.0
1	A	484	ALA	3.0
1	C	336	ALA	2.9
1	C	360	VAL	2.9
1	A	719	ILE	2.9
1	A	488	GLU	2.8
1	A	830	ASP	2.8
1	A	333	ILE	2.8
1	A	489	LYS	2.8
1	C	345	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	356	ASN	2.8
1	A	520	LEU	2.8
1	A	335	GLU	2.8
1	C	361	LEU	2.7
1	A	318	ASP	2.7
1	A	739	PRO	2.7
1	C	763	ASN	2.7
1	C	1028	LYS	2.6
1	A	770	ASN	2.6
1	A	328	ARG	2.6
1	C	609	PRO	2.5
1	A	541	LEU	2.5
1	A	332	ASN	2.5
1	C	353	ALA	2.5
1	C	739	PRO	2.4
1	A	895	VAL	2.4
1	C	742	LYS	2.4
1	A	892	PHE	2.4
1	A	480	VAL	2.4
1	C	527	VAL	2.4
1	C	895	VAL	2.3
1	A	320	LEU	2.3
1	C	830	ASP	2.3
1	A	531	PRO	2.2
1	A	485	ASP	2.2
1	A	537	LYS	2.2
1	C	450	PRO	2.2
1	C	531	PRO	2.2
1	C	447	LYS	2.2
1	A	346	VAL	2.2
1	C	491	ARG	2.2
1	A	771	THR	2.2
1	A	860	ASN	2.2
1	A	350	PHE	2.2
1	A	506	SER	2.1
1	A	712	ASP	2.1
1	A	774	GLU	2.1
1	A	483	VAL	2.0
1	A	896	ALA	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)

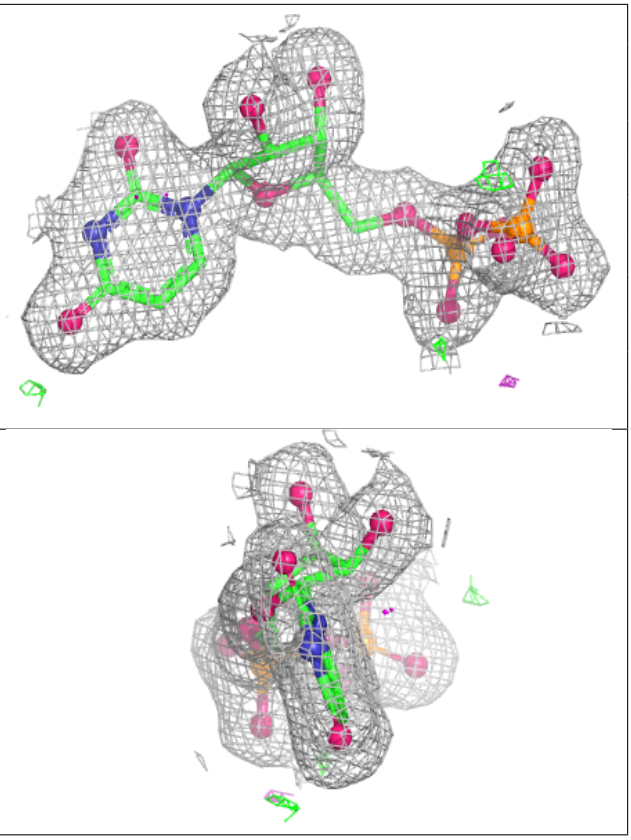
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

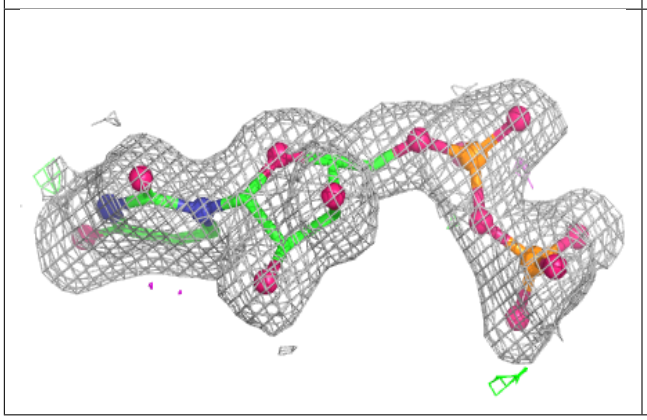
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	1102	5/5	0.86	0.22	66,66,66,67	0
5	0YT	B	101	14/15	0.93	0.11	14,20,29,31	0
5	0YT	D	101	14/15	0.93	0.15	14,19,28,31	0
4	SO4	B	102	5/5	0.97	0.12	41,42,45,45	0
4	SO4	D	102	5/5	0.97	0.17	41,43,45,47	0
3	UDP	C	1101	25/25	0.98	0.12	10,14,16,18	0
3	UDP	A	1101	25/25	0.98	0.10	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.

Electron density around UDP C 1101:

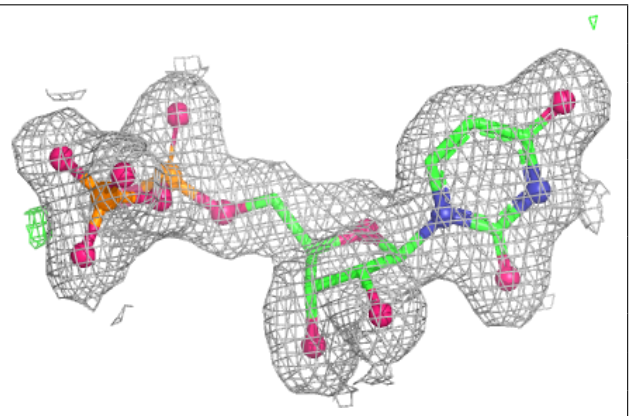
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

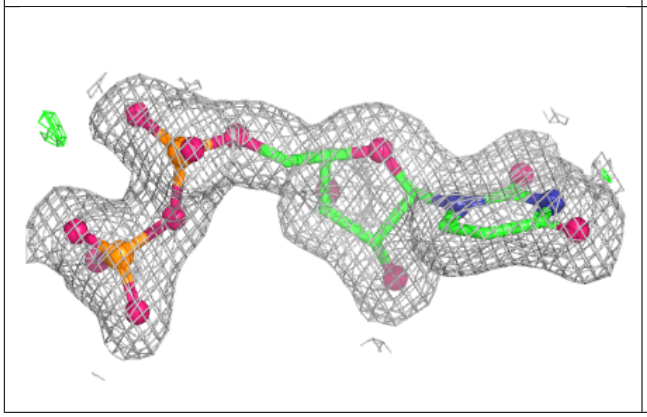


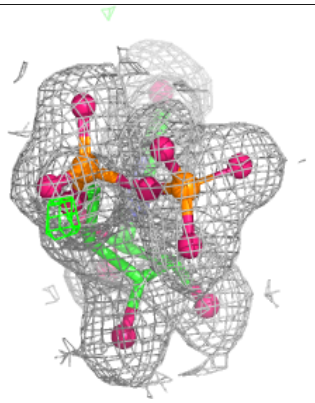


Electron density around UDP A 1101:

$2mF_o$-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.