



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 05:48 AM BST

PDB ID : 5LVV
Title : Human OGT in complex with UDP and fused substrate peptide (Tab1)
Authors : Raimi, O.
Deposited on : 2016-09-14
Resolution : 2.54 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

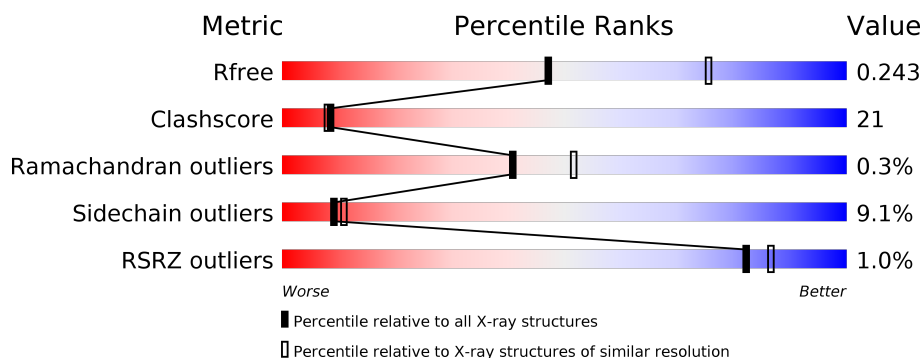
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 on 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	749	<div> <div> <div></div> <div>66%</div> <div>26%</div> <div></div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5771 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.

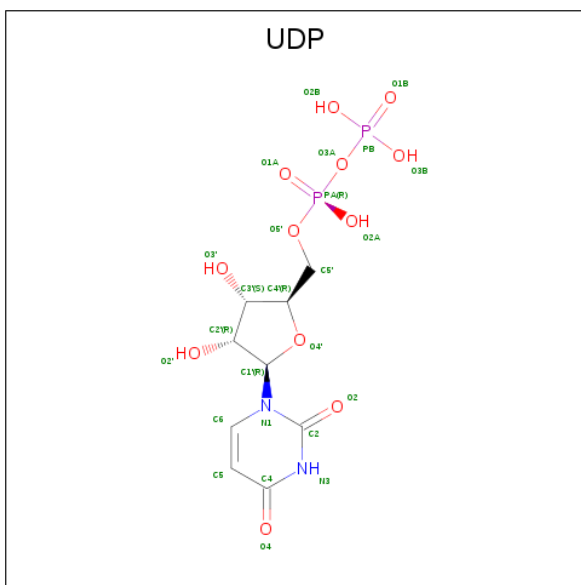
- Molecule 1 is a protein called UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit,UDP-N-acetylglucosamine--peptide N-acetylglucosaminyltransferase 110 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	720	Total	C	N	O	S	0	0	0
			5664	3588	994	1046	36			

There are 9 discrepancies between the modelled and reference sequences:

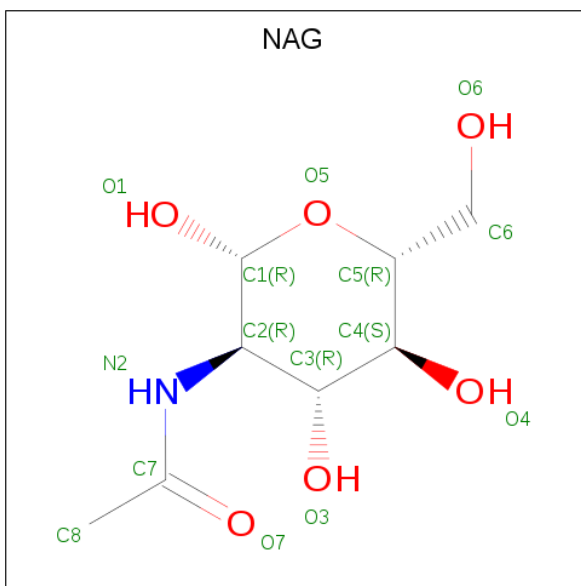
Chain	Residue	Modelled	Actual	Comment	Reference
A	288	HIS	-	expression tag	PDB ?
A	289	HIS	-	expression tag	PDB ?
A	290	HIS	-	expression tag	PDB ?
A	291	HIS	-	expression tag	PDB ?
A	292	HIS	-	expression tag	PDB ?
A	293	HIS	-	expression tag	PDB ?
A	312	GLY	-	linker	PDB ?
A	313	GLY	-	linker	PDB ?
A	314	GLY	-	linker	PDB ?

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.53 Å 98.53 Å 367.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.70 – 2.54 49.73 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.70-2.54) 99.8 (49.73-2.54)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.54 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.193 , 0.245 0.208 , 0.243	Depositor DCC
R_{free} test set	1795 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.5	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	5771	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: UDP, NAG

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	1.03	0/5796	0.70	2/7862 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	919	GLY	N-CA-C	-5.75	98.74	113.10
1	A	714	LYS	N-CA-C	5.03	124.58	111.00

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	5664	0	5615	236	0
2	A	25	0	11	0	0
3	A	42	0	39	8	0
4	A	40	0	0	1	0
All	All	5771	0	5665	236	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 21.

All (236) 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:A:301:SER:CB	3:A:1204:NAG:C1	1.83	1.56
1:A:301:SER:OG	3:A:1204:NAG:C2	1.63	1.45
1:A:745:LYS:CB	1:A:763:ASN:HD22	1.30	1.44
1:A:745:LYS:CB	1:A:763:ASN:HB3	1.54	1.38
1:A:745:LYS:HB3	1:A:763:ASN:ND2	1.46	1.30
1:A:587:ASP:OD1	1:A:589:THR:OG1	1.54	1.19
1:A:745:LYS:CB	1:A:763:ASN:ND2	2.02	1.18
1:A:745:LYS:HB3	1:A:763:ASN:CB	1.72	1.16
1:A:745:LYS:CB	1:A:763:ASN:CB	2.23	1.16
1:A:745:LYS:CA	1:A:763:ASN:HB3	1.77	1.14
1:A:884:GLY:HA3	1:A:885:LEU:HB2	1.27	1.12
1:A:301:SER:OG	3:A:1204:NAG:C1	0.83	1.12
1:A:630:ASN:O	1:A:633:THR:OG1	1.64	1.10
1:A:669:THR:HG21	1:A:674:SER:OG	1.49	1.10
1:A:745:LYS:CG	1:A:763:ASN:HD22	1.65	1.10
1:A:745:LYS:HB3	1:A:763:ASN:CG	1.73	1.07
1:A:884:GLY:CA	1:A:885:LEU:HB2	1.84	1.06
1:A:677:GLU:N	1:A:677:GLU:OE2	1.90	1.05
1:A:616:ASP:O	1:A:620:GLN:HG3	1.56	1.03
1:A:744:VAL:O	1:A:763:ASN:HB2	1.57	1.02
1:A:957:GLU:OE2	1:A:986:LYS:HE2	1.59	1.00
1:A:693:PHE:O	1:A:1002:TYR:OH	1.80	0.98
1:A:1011:LEU:O	1:A:1015:GLU:HG2	1.65	0.97
1:A:745:LYS:HA	1:A:763:ASN:HB3	1.45	0.96
1:A:714:LYS:HD3	1:A:717:GLY:O	1.65	0.96
1:A:301:SER:HB3	3:A:1204:NAG:C1	1.98	0.94
1:A:963:ARG:O	1:A:967:GLU:HG3	1.66	0.94
1:A:778:GLU:OE2	1:A:782:ARG:HD2	1.68	0.93
1:A:301:SER:OG	3:A:1204:NAG:N2	2.01	0.93
1:A:658:THR:OG1	1:A:684:GLU:OE1	1.87	0.91
1:A:745:LYS:HB2	1:A:763:ASN:HB3	1.51	0.90
1:A:986:LYS:O	1:A:990:GLN:CG	2.24	0.85
1:A:1027:ILE:HD13	1:A:1027:ILE:H	1.42	0.83
1:A:717:GLY:O	1:A:718:HIS:HB2	1.76	0.83
1:A:972:LYS:HD3	1:A:979:TYR:CD2	2.16	0.81
1:A:538:ASP:CG	1:A:540:LYS:HD3	2.02	0.80
1:A:745:LYS:HG3	1:A:763:ASN:HD22	1.45	0.79
1:A:295:PRO:HG3	1:A:557:ASN:O	1.83	0.77
1:A:986:LYS:O	1:A:990:GLN:HG2	1.84	0.77
1:A:1027:ILE:C	1:A:1028:LYS:HD3	2.03	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:LYS:CA	1:A:763:ASN:CB	2.59	0.76
1:A:617:ARG:HD2	1:A:617:ARG:O	1.86	0.75
1:A:321:ASN:HD21	1:A:356:ASN:HD22	1.33	0.75
1:A:884:GLY:HA3	1:A:885:LEU:CB	2.05	0.75
1:A:538:ASP:OD1	1:A:540:LYS:HB2	1.87	0.74
1:A:327:LYS:HD2	1:A:335:GLU:HG2	1.68	0.74
1:A:536:PRO:C	1:A:537:LYS:HD3	2.08	0.74
1:A:522:LEU:N	1:A:522:LEU:HD23	2.03	0.73
1:A:986:LYS:O	1:A:990:GLN:HG3	1.88	0.73
1:A:541:LEU:HD23	1:A:541:LEU:N	2.03	0.73
1:A:714:LYS:N	1:A:715:SER:HA	2.01	0.73
1:A:603:ILE:N	1:A:603:ILE:HD12	2.04	0.73
1:A:738:LEU:HD22	1:A:772:ILE:HD12	1.72	0.72
1:A:712:ASP:OD2	1:A:715:SER:O	2.07	0.71
1:A:334:GLU:CD	1:A:334:GLU:H	1.93	0.70
1:A:611:ASN:ND2	1:A:639:GLU:HB2	2.07	0.70
1:A:509:PHE:O	1:A:513:ILE:HG13	1.91	0.69
1:A:398:MET:C	1:A:399:GLN:HG2	2.13	0.69
1:A:611:ASN:ND2	1:A:639:GLU:CB	2.56	0.69
1:A:716:ASN:H	1:A:716:ASN:ND2	1.90	0.69
1:A:778:GLU:CD	1:A:782:ARG:HD2	2.14	0.68
1:A:941:LEU:O	1:A:941:LEU:HD23	1.93	0.68
1:A:1028:LYS:C	1:A:1028:LYS:HE3	2.14	0.68
1:A:745:LYS:HB2	1:A:763:ASN:ND2	2.07	0.67
1:A:734:PHE:O	1:A:737:SER:OG	2.12	0.67
1:A:745:LYS:HA	1:A:763:ASN:CB	2.21	0.67
1:A:745:LYS:CB	1:A:763:ASN:CG	2.48	0.66
1:A:778:GLU:O	1:A:782:ARG:HG3	1.95	0.66
1:A:745:LYS:HG3	1:A:763:ASN:ND2	2.09	0.66
1:A:611:ASN:OD1	1:A:637:ARG:NH2	2.23	0.65
1:A:712:ASP:OD1	1:A:719:ILE:HG12	1.97	0.65
1:A:716:ASN:HD22	1:A:716:ASN:H	1.44	0.65
1:A:535:HIS:O	1:A:537:LYS:CE	2.44	0.65
1:A:842:LYS:HG2	1:A:917:CYS:HB3	1.79	0.64
1:A:745:LYS:N	1:A:745:LYS:HD2	2.12	0.64
1:A:1027:ILE:H	1:A:1027:ILE:CD1	2.10	0.63
1:A:745:LYS:CG	1:A:763:ASN:ND2	2.48	0.63
1:A:538:ASP:OD1	1:A:540:LYS:HD3	1.99	0.62
1:A:616:ASP:O	1:A:620:GLN:CG	2.41	0.62
1:A:714:LYS:CD	1:A:717:GLY:O	2.43	0.62
1:A:376:GLU:O	1:A:380:ILE:HG13	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:ILE:O	1:A:1028:LYS:HD3	2.00	0.62
1:A:884:GLY:N	1:A:885:LEU:HB2	2.17	0.60
1:A:461:HIS:NE2	1:A:499:HIS:CD2	2.69	0.60
1:A:941:LEU:HD23	1:A:941:LEU:C	2.21	0.60
1:A:557:ASN:HB2	1:A:589:THR:HG21	1.84	0.60
1:A:1010:TYR:O	1:A:1013:MET:HB2	2.02	0.60
1:A:712:ASP:O	1:A:715:SER:CB	2.50	0.60
1:A:690:PRO:HG3	1:A:1005:GLU:OE1	2.02	0.59
1:A:333:ILE:O	1:A:337:VAL:HG23	2.02	0.59
1:A:744:VAL:O	1:A:764:MET:N	2.33	0.59
1:A:579:PHE:CE2	1:A:601:HIS:CD2	2.91	0.59
1:A:741:VAL:HG22	1:A:767:ILE:HG12	1.85	0.58
1:A:726:LEU:CD1	1:A:819:VAL:HG22	2.32	0.58
1:A:660:GLY:HA2	1:A:683:SER:HB3	1.84	0.58
1:A:884:GLY:CA	1:A:885:LEU:CB	2.67	0.58
1:A:714:LYS:HD3	1:A:718:HIS:HB2	1.86	0.57
1:A:360:VAL:O	1:A:364:GLN:HG3	2.04	0.57
1:A:744:VAL:O	1:A:763:ASN:CB	2.42	0.57
1:A:398:MET:O	1:A:399:GLN:CB	2.53	0.57
1:A:535:HIS:O	1:A:537:LYS:HE2	2.05	0.56
1:A:617:ARG:HH11	1:A:617:ARG:HG2	1.70	0.56
1:A:667:ILE:HG23	1:A:667:ILE:O	2.05	0.56
1:A:1028:LYS:N	1:A:1028:LYS:HD3	2.18	0.56
1:A:602:PHE:C	1:A:603:ILE:HD12	2.25	0.56
1:A:938:GLY:O	1:A:944:ARG:HD2	2.05	0.56
1:A:486:GLN:OE1	1:A:493:PRO:HA	2.06	0.56
1:A:712:ASP:O	1:A:715:SER:HB3	2.06	0.56
1:A:1025:HIS:CD2	1:A:1025:HIS:H	2.23	0.55
1:A:340:TYR:CZ	1:A:356:ASN:HB3	2.41	0.55
1:A:1027:ILE:N	1:A:1027:ILE:HD13	2.16	0.54
1:A:301:SER:CB	3:A:1204:NAG:O5	2.52	0.54
1:A:773:ALA:O	1:A:777:ILE:HG23	2.08	0.54
1:A:617:ARG:NH1	1:A:617:ARG:HG2	2.22	0.54
1:A:384:PHE:CE1	1:A:386:ASP:HB2	2.42	0.54
1:A:745:LYS:HD2	1:A:745:LYS:H	1.74	0.53
1:A:651:MET:HG2	1:A:664:MET:HE2	1.90	0.53
1:A:536:PRO:O	1:A:537:LYS:HD3	2.09	0.53
1:A:770:ASN:HB3	1:A:773:ALA:H	1.74	0.53
1:A:333:ILE:HD13	1:A:333:ILE:N	2.23	0.52
1:A:538:ASP:OD1	1:A:540:LYS:N	2.38	0.52
1:A:745:LYS:N	1:A:745:LYS:CD	2.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:972:LYS:HD3	1:A:979:TYR:CE2	2.45	0.52
1:A:596:MET:HG2	1:A:602:PHE:CD1	2.45	0.52
1:A:644:ARG:N	1:A:645:PRO:CD	2.73	0.52
1:A:533:TYR:CD1	1:A:619:HIS:CG	2.98	0.52
1:A:695:ILE:HG13	1:A:696:GLY:N	2.25	0.52
1:A:910:VAL:HG12	1:A:911:CYS:N	2.24	0.51
1:A:690:PRO:HG3	1:A:1005:GLU:CD	2.31	0.51
1:A:326:ILE:O	1:A:330:GLN:HG3	2.12	0.50
1:A:533:TYR:OH	1:A:616:ASP:OD1	2.23	0.50
1:A:340:TYR:CE1	1:A:356:ASN:HB3	2.47	0.50
1:A:430:LYS:HD2	1:A:462:CYS:SG	2.51	0.50
1:A:473:ASP:OD2	1:A:474:GLU:N	2.43	0.50
1:A:745:LYS:HB2	1:A:763:ASN:CB	2.24	0.50
1:A:547:ARG:HB2	1:A:624:HIS:CE1	2.46	0.50
1:A:545:ARG:NH1	1:A:576:PHE:O	2.46	0.49
1:A:292:HIS:C	1:A:292:HIS:CD2	2.85	0.49
1:A:712:ASP:O	1:A:715:SER:HB2	2.11	0.49
1:A:408:TYR:O	1:A:412:ILE:HG12	2.13	0.49
1:A:368:GLN:OE1	1:A:368:GLN:HA	2.13	0.49
1:A:549:GLY:HA2	1:A:579:PHE:O	2.13	0.49
1:A:844:ASP:HB2	1:A:845:PRO:CD	2.42	0.49
1:A:738:LEU:HD22	1:A:772:ILE:CD1	2.42	0.48
1:A:716:ASN:N	1:A:716:ASN:ND2	2.60	0.48
1:A:558:HIS:CG	1:A:559:PRO:HD2	2.48	0.48
1:A:533:TYR:HD1	1:A:619:HIS:CG	2.32	0.48
1:A:398:MET:O	1:A:399:GLN:HB2	2.13	0.48
1:A:485:ASP:O	1:A:489:LYS:HG3	2.13	0.48
1:A:844:ASP:HB2	1:A:845:PRO:HD2	1.96	0.48
1:A:685:LYS:HD2	1:A:1025:HIS:CD2	2.48	0.48
1:A:611:ASN:HD22	1:A:639:GLU:CB	2.25	0.48
1:A:714:LYS:HD3	1:A:718:HIS:CB	2.44	0.47
1:A:473:ASP:OD2	1:A:473:ASP:N	2.46	0.47
1:A:1027:ILE:N	1:A:1027:ILE:CD1	2.73	0.47
1:A:742:LYS:HB2	1:A:742:LYS:HE2	1.59	0.47
1:A:603:ILE:HG22	1:A:605:LEU:HD23	1.96	0.47
1:A:479:LEU:O	1:A:483:VAL:HG23	2.15	0.47
1:A:805:ASN:ND2	1:A:805:ASN:H	2.13	0.47
1:A:295:PRO:HA	4:A:1334:HOH:O	2.14	0.47
1:A:537:LYS:HD3	1:A:537:LYS:N	2.28	0.47
1:A:729:ILE:HA	1:A:729:ILE:HD13	1.74	0.47
1:A:740:ASP:OD2	1:A:740:ASP:N	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:ILE:HD13	1:A:970:ALA:CB	2.45	0.47
1:A:396:LYS:HG3	1:A:428:ILE:HD11	1.97	0.46
1:A:408:TYR:CZ	1:A:424:ASN:HB3	2.51	0.46
1:A:732:LYS:HE3	1:A:736:ASP:OD2	2.15	0.46
1:A:624:HIS:O	1:A:647:PRO:HG2	2.15	0.46
1:A:304:LYS:HE3	1:A:305:THR:O	2.16	0.46
1:A:952:CYS:SG	1:A:995:PRO:HG2	2.56	0.46
1:A:674:SER:O	1:A:688:TYR:OH	2.17	0.45
1:A:608:ILE:N	1:A:609:PRO:CD	2.80	0.45
1:A:714:LYS:N	1:A:715:SER:CA	2.78	0.45
1:A:627:VAL:CG1	1:A:652:TRP:HB3	2.46	0.45
1:A:885:LEU:HD12	1:A:885:LEU:HA	1.70	0.45
1:A:590:ASN:HB2	1:A:811:GLU:HG2	1.99	0.45
1:A:896:ALA:HB1	1:A:897:PRO:HD2	1.99	0.45
1:A:398:MET:C	1:A:399:GLN:CG	2.78	0.45
1:A:533:TYR:HD1	1:A:619:HIS:CD2	2.35	0.44
1:A:490:ASN:HA	1:A:516:ARG:NH1	2.33	0.44
1:A:490:ASN:HA	1:A:516:ARG:HH12	1.83	0.44
1:A:644:ARG:N	1:A:645:PRO:HD2	2.32	0.44
1:A:732:LYS:CE	1:A:736:ASP:OD2	2.65	0.44
1:A:821:THR:O	1:A:824:GLN:HB2	2.17	0.44
1:A:737:SER:O	1:A:739:PRO:HD3	2.17	0.44
1:A:561:SER:O	1:A:565:GLN:HG2	2.18	0.44
1:A:967:GLU:O	1:A:971:VAL:HG23	2.18	0.44
1:A:398:MET:O	1:A:399:GLN:CG	2.66	0.44
1:A:744:VAL:C	1:A:763:ASN:HB2	2.32	0.43
1:A:292:HIS:O	1:A:292:HIS:CD2	2.70	0.43
1:A:990:GLN:HB3	1:A:990:GLN:HE21	1.64	0.43
1:A:298:SER:OG	3:A:1203:NAG:C6	2.63	0.43
1:A:611:ASN:ND2	1:A:639:GLU:HB3	2.34	0.43
1:A:941:LEU:CD2	1:A:941:LEU:C	2.85	0.43
1:A:333:ILE:HG23	1:A:360:VAL:CG1	2.49	0.43
1:A:1025:HIS:N	1:A:1025:HIS:CD2	2.87	0.43
1:A:852:ALA:O	1:A:856:LYS:HG3	2.18	0.43
1:A:523:ASP:N	1:A:523:ASP:OD1	2.51	0.43
1:A:461:HIS:CD2	1:A:499:HIS:CD2	3.07	0.43
1:A:1028:LYS:C	1:A:1028:LYS:CE	2.87	0.42
1:A:603:ILE:CD1	1:A:603:ILE:N	2.73	0.42
1:A:745:LYS:H	1:A:745:LYS:CD	2.32	0.42
1:A:1011:LEU:HD23	1:A:1011:LEU:HA	1.79	0.42
1:A:547:ARG:NE	1:A:577:GLU:OE1	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:LYS:C	1:A:989:LYS:HD2	2.39	0.42
1:A:714:LYS:NZ	1:A:720:TYR:HE2	2.16	0.42
1:A:738:LEU:CD2	1:A:772:ILE:CD1	2.97	0.42
1:A:1016:HIS:NE2	1:A:1021:ASN:HB3	2.33	0.42
1:A:604:ASP:C	1:A:606:SER:H	2.23	0.42
1:A:669:THR:HG22	1:A:670:ASP:H	1.85	0.42
1:A:805:ASN:ND2	1:A:805:ASN:N	2.67	0.42
1:A:547:ARG:H	1:A:624:HIS:CE1	2.38	0.42
1:A:292:HIS:O	1:A:292:HIS:HD2	2.03	0.42
1:A:1027:ILE:O	1:A:1027:ILE:HG12	2.20	0.42
1:A:611:ASN:HD22	1:A:639:GLU:HB3	1.84	0.42
1:A:725:VAL:HG12	1:A:726:LEU:N	2.35	0.42
1:A:579:PHE:CD1	1:A:579:PHE:N	2.87	0.42
1:A:714:LYS:NZ	1:A:720:TYR:CE2	2.87	0.41
1:A:855:LEU:O	1:A:889:ARG:NH2	2.50	0.41
1:A:717:GLY:O	1:A:718:HIS:CB	2.55	0.41
1:A:854:ILE:HD13	1:A:970:ALA:HB3	2.01	0.41
1:A:889:ARG:HA	1:A:889:ARG:HD2	1.87	0.41
1:A:681:GLN:HG2	1:A:681:GLN:O	2.20	0.41
1:A:738:LEU:HA	1:A:739:PRO:HD3	1.86	0.41
1:A:572:ASN:HA	1:A:573:PRO:HD3	1.87	0.41
1:A:522:LEU:HD23	1:A:522:LEU:H	1.80	0.41
1:A:839:GLN:OE1	3:A:1203:NAG:H82	2.20	0.41
1:A:533:TYR:CD1	1:A:619:HIS:CD2	3.09	0.41
1:A:310:SER:O	1:A:311:LEU:HD23	2.21	0.41
1:A:356:ASN:O	1:A:360:VAL:HG23	2.21	0.41
1:A:589:THR:O	1:A:593:VAL:HG23	2.20	0.41
1:A:542:SER:O	1:A:543:ASP:CB	2.67	0.41
1:A:694:PHE:CZ	1:A:920:HIS:HB3	2.56	0.40
1:A:805:ASN:N	1:A:805:ASN:HD22	2.18	0.40
1:A:546:LEU:HA	1:A:546:LEU:HD12	1.90	0.40
1:A:685:LYS:HD2	1:A:1025:HIS:NE2	2.35	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	716/749 (96%)	702 (98%)	12 (2%)	2 (0%)	41 51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	885	LEU
1	A	718	HIS

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	615/641 (96%)	559 (91%)	56 (9%)	9 11

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	HIS
1	A	306	SER
1	A	315	THR
1	A	316	HIS
1	A	334	GLU
1	A	345	GLU
1	A	350	PHE
1	A	372	MET
1	A	443	ARG
1	A	452	PHE
1	A	489	LYS
1	A	490	ASN
1	A	491	ARG
1	A	522	LEU
1	A	540	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	541	LEU
1	A	547	ARG
1	A	589	THR
1	A	606	SER
1	A	633	THR
1	A	634	LYS
1	A	669	THR
1	A	677	GLU
1	A	680	GLU
1	A	694	PHE
1	A	714	LYS
1	A	716	ASN
1	A	718	HIS
1	A	745	LYS
1	A	763	ASN
1	A	770	ASN
1	A	771	THR
1	A	777	ILE
1	A	778	GLU
1	A	784	GLN
1	A	805	ASN
1	A	806	LYS
1	A	821	THR
1	A	823	SER
1	A	829	GLU
1	A	830	ASP
1	A	855	LEU
1	A	856	LYS
1	A	868	PHE
1	A	881	GLN
1	A	888	ASN
1	A	893	SER
1	A	914	THR
1	A	926	VAL
1	A	989	LYS
1	A	990	GLN
1	A	994	SER
1	A	1000	LYS
1	A	1008	ARG
1	A	1027	ILE
1	A	1028	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	HIS
1	A	321	ASN
1	A	363	GLN
1	A	402	GLN
1	A	422	HIS
1	A	498	HIS
1	A	517	HIS
1	A	601	HIS
1	A	716	ASN
1	A	763	ASN
1	A	805	ASN
1	A	878	GLN
1	A	887	GLN
1	A	990	GLN
1	A	1025	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	NAG	A	1202	1	14,14,15	0.88	0	17,19,21	1.68	1 (5%)
2	UDP	A	1201	-	20,26,26	1.19	2 (10%)	25,40,40	1.40	3 (12%)
3	NAG	A	1203	-	14,14,15	1.53	3 (21%)	17,19,21	2.93	11 (64%)
3	NAG	A	1204	-	14,14,15	0.89	0	17,19,21	1.92	4 (23%)

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	NAG	A	1202	1	-	0/6/23/26	0/1/1/1
2	UDP	A	1201	-	-	4/14/32/32	0/2/2/2
3	NAG	A	1203	-	-	2/6/23/26	0/1/1/1
3	NAG	A	1204	-	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	UDP	C2'-C1'	-3.44	1.48	1.53
3	A	1203	NAG	C2-N2	3.08	1.51	1.46
3	A	1203	NAG	C1-C2	2.75	1.56	1.52
3	A	1203	NAG	C3-C2	2.37	1.57	1.52
2	A	1201	UDP	C2-N3	-2.16	1.33	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1203	NAG	O5-C5-C6	8.60	120.69	107.20
3	A	1202	NAG	C1-O5-C5	6.04	120.38	112.19
3	A	1204	NAG	C2-N2-C7	4.59	129.43	122.90
3	A	1204	NAG	C4-C3-C2	-3.49	105.91	111.02
3	A	1203	NAG	O7-C7-C8	-3.44	115.67	122.06
2	A	1201	UDP	O2A-PA-O1A	3.26	128.35	112.24
3	A	1203	NAG	O5-C1-C2	-3.14	106.33	111.29
3	A	1203	NAG	C1-C2-N2	3.04	115.69	110.49
2	A	1201	UDP	O3B-PB-O3A	-2.99	94.59	104.64
3	A	1203	NAG	C8-C7-N2	2.82	120.87	116.10
3	A	1204	NAG	O3-C3-C2	2.40	114.42	109.47
2	A	1201	UDP	O3B-PB-O1B	2.36	119.91	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1203	NAG	O4-C4-C5	-2.26	103.67	109.30
3	A	1204	NAG	O4-C4-C5	2.26	114.91	109.30
3	A	1203	NAG	O4-C4-C3	2.25	115.56	110.35
3	A	1203	NAG	C3-C4-C5	2.23	114.22	110.24
3	A	1203	NAG	C1-O5-C5	2.21	115.19	112.19
3	A	1203	NAG	O5-C5-C4	-2.03	105.88	110.83
3	A	1203	NAG	O3-C3-C4	-2.03	105.66	110.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

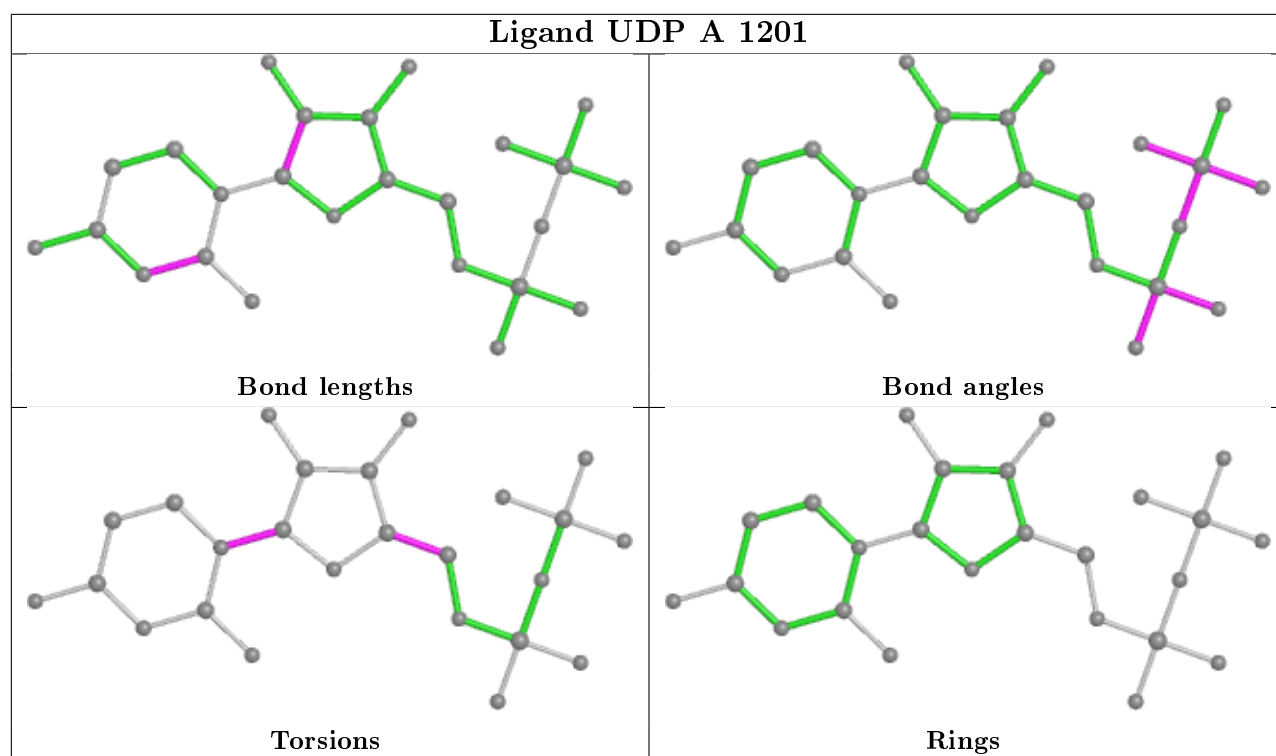
Mol	Chain	Res	Type	Atoms
2	A	1201	UDP	C2'-C1'-N1-C6
2	A	1201	UDP	O4'-C1'-N1-C6
3	A	1204	NAG	C3-C2-N2-C7
3	A	1204	NAG	O5-C5-C6-O6
3	A	1204	NAG	C4-C5-C6-O6
3	A	1203	NAG	O5-C5-C6-O6
2	A	1201	UDP	O4'-C4'-C5'-O5'
2	A	1201	UDP	C3'-C4'-C5'-O5'
3	A	1203	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1203	NAG	2	0
3	A	1204	NAG	6	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	720/749 (96%)	-0.05	7 (0%) 82 86	47, 68, 105, 157	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	LEU	4.0
1	A	312	GLY	3.8
1	A	715	SER	3.7
1	A	716	ASN	3.7
1	A	292	HIS	3.2
1	A	544	GLY	2.6
1	A	714	LYS	2.5

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 monosaccharides 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.

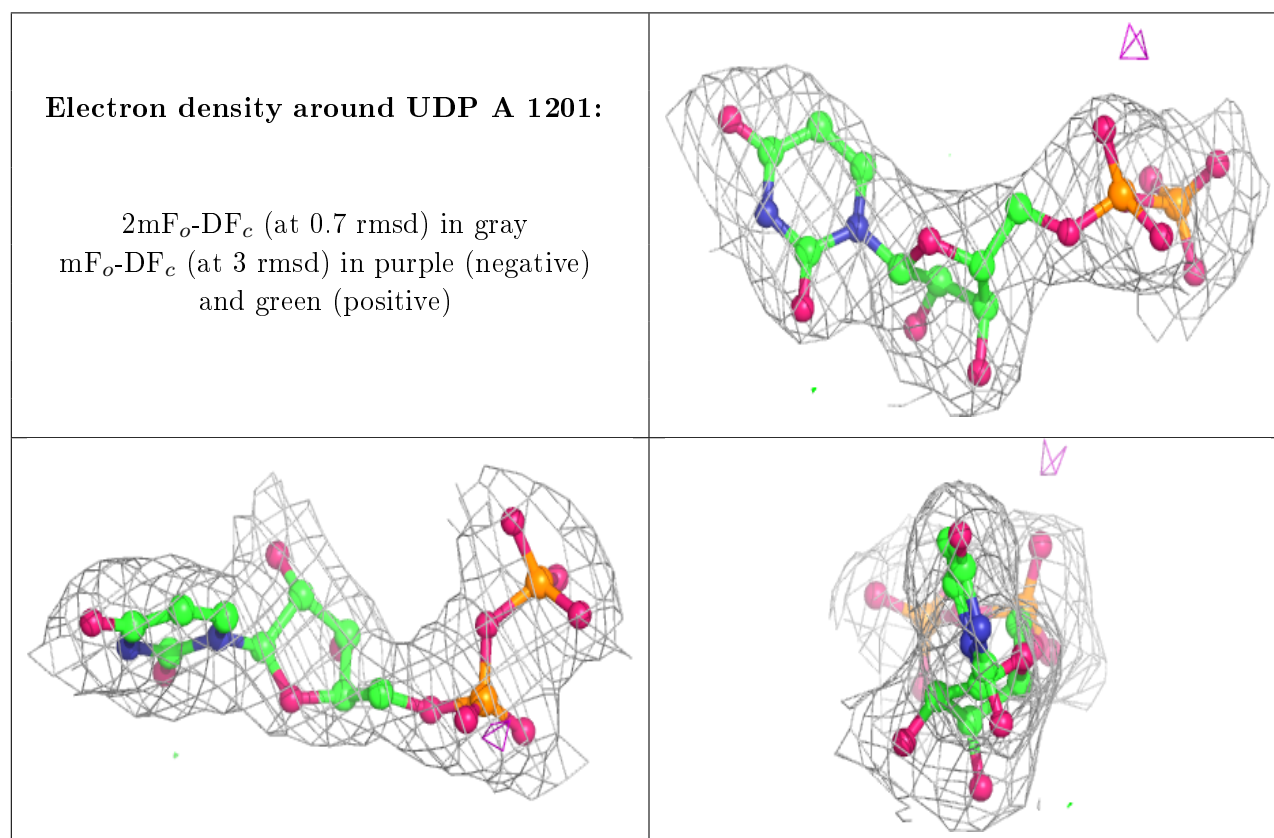
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	1203	14/15	0.89	0.29	70,83,97,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	1204	14/15	0.96	0.18	73,83,91,96	0
3	NAG	A	1202	14/15	0.97	0.20	50,56,60,60	0
2	UDP	A	1201	25/25	0.99	0.19	44,48,54,57	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.