



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 04:09 pm BST

PDB ID : 8P0P
Title : Crystal structure of AaNGT complexed to UDP-2F-Glucose
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Deposited on : 2023-05-10
Resolution : 2.73 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

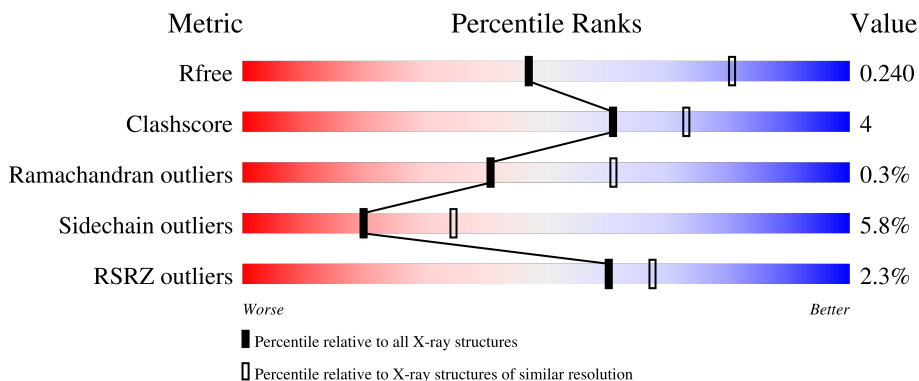
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	622	 % 82% 17% .
1	B	622	 4% 85% 14% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10035 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.

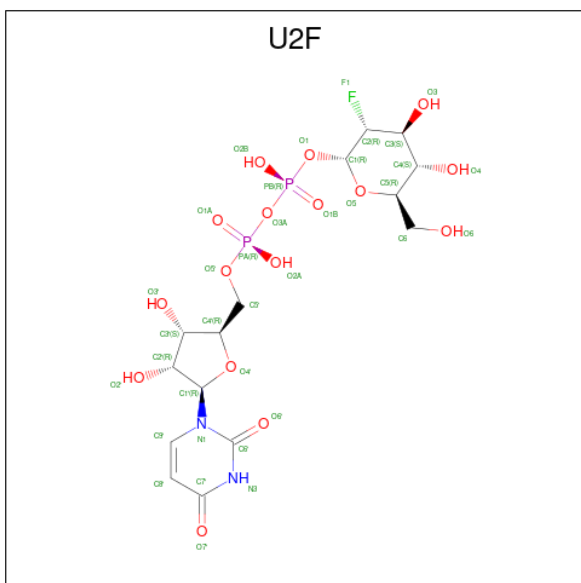
- Molecule 1 is a protein called Adhesin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	622	Total 4983	C 3181	N 849	O 924	S 29	0	0	0
1	B	622	Total 4983	C 3181	N 849	O 924	S 29	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

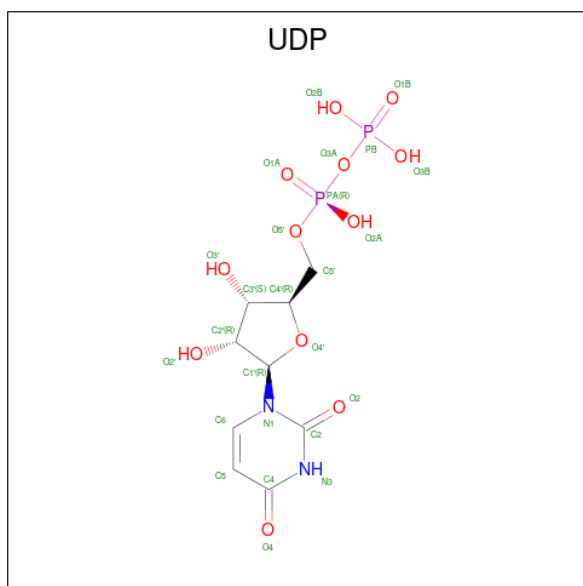
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A3M6PNT1
A	3	ARG	GLU	conflict	UNP A0A3M6PNT1
B	0	GLY	-	expression tag	UNP A0A3M6PNT1
B	3	ARG	GLU	conflict	UNP A0A3M6PNT1

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-2-DEOXY-2-FLUORO-ALPHA-D-GLUCOSE (three-letter code: U2F) (formula: C₁₅H₂₃FN₂O₁₆P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			P
2	A	1	36	15	1	2	16	2	0	0

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂) (labeled as "Ligand of Interest" by depositor).



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

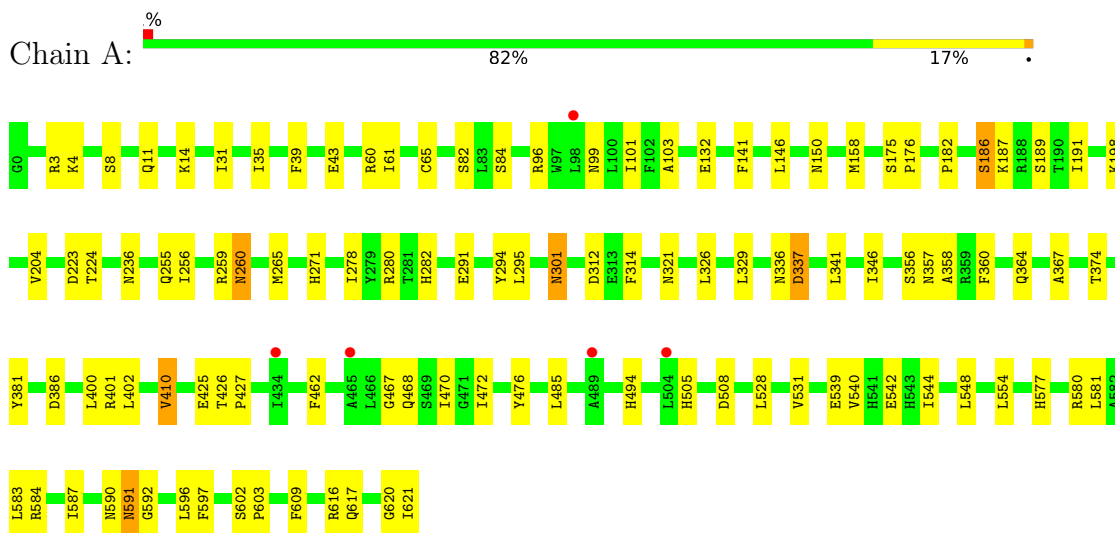
- Molecule 4 is water.

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

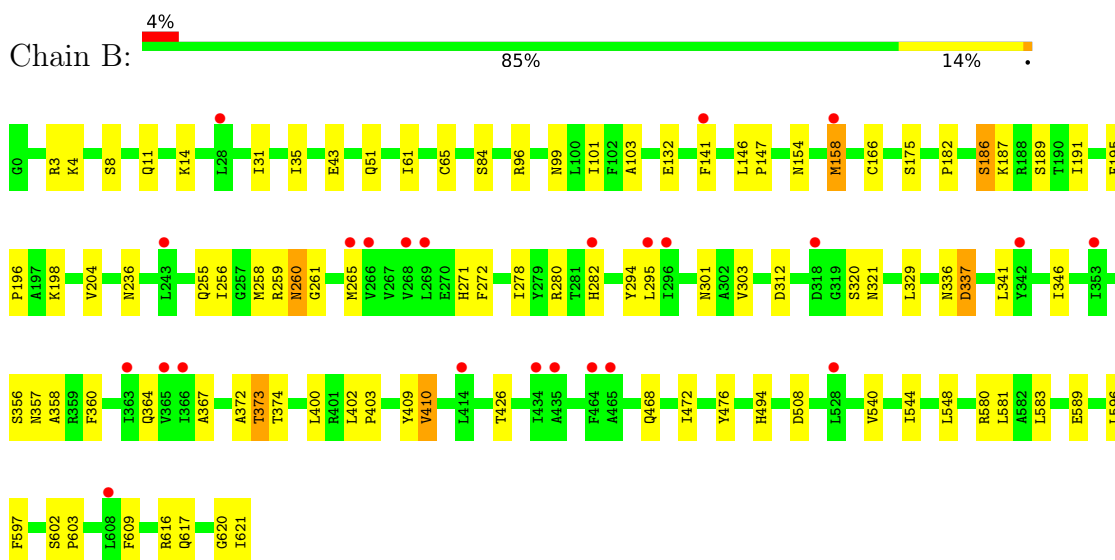
3 Residue-property plots [i](#)

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: Adhesin



- Molecule 1: Adhesin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.07Å 114.00Å 258.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	129.00 – 2.73 129.00 – 2.73	Depositor EDS
% Data completeness (in resolution range)	100.0 (129.00-2.73) 100.0 (129.00-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.73Å)	Xtrriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.197 , 0.245 0.200 , 0.240	Depositor DCC
R_{free} test set	1430 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å ²)	85.2	Xtrriage
Anisotropy	0.479	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10035	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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, U2F

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	0.37	0/5104	0.72	0/6927
1	B	0.36	0/5104	0.70	0/6927
All	All	0.36	0/10208	0.71	0/13854

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ARG	Sidechain

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	4983	0	4903	50	0
1	B	4983	0	4903	41	0
2	A	36	0	21	0	0
3	B	25	0	11	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
All	All	10035	0	9838	89	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 4.

All (89) 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:150:ASN:ND2	1:B:51:GLN:HE21	1.87	0.73
1:A:150:ASN:HD21	1:B:51:GLN:HE21	1.45	0.65
1:A:508:ASP:O	1:A:580:ARG:HD3	1.98	0.64
1:A:346:ILE:CD1	1:A:356:SER:HB3	2.28	0.62
1:A:540:VAL:O	1:A:544:ILE:HG13	1.99	0.62
1:B:540:VAL:O	1:B:544:ILE:HG13	2.00	0.60
1:B:346:ILE:CD1	1:B:356:SER:HB3	2.33	0.57
1:B:508:ASP:O	1:B:580:ARG:HD3	2.05	0.57
1:B:271:HIS:O	1:B:278:ILE:HG21	2.05	0.57
1:A:301:ASN:H	1:A:301:ASN:ND2	2.03	0.56
1:A:590:ASN:O	1:A:592:GLY:N	2.38	0.56
1:B:468:GLN:H	1:B:494:HIS:HD2	1.55	0.55
1:A:602:SER:N	1:A:603:PRO:CD	2.71	0.54
1:B:258:MET:CE	1:B:261:GLY:O	2.56	0.54
1:B:602:SER:N	1:B:603:PRO:CD	2.72	0.53
1:A:236:ASN:ND2	1:A:374:THR:O	2.42	0.53
1:A:265:MET:HE2	1:A:295:LEU:HD11	1.91	0.53
1:B:236:ASN:ND2	1:B:374:THR:O	2.42	0.53
1:B:294:TYR:CE1	1:B:312:ASP:HB3	2.44	0.53
1:A:182:PRO:O	1:A:186:SER:HB3	2.09	0.52
1:B:616:ARG:O	1:B:620:GLY:HA2	2.10	0.52
1:B:282:HIS:CE1	1:B:367:ALA:HB1	2.44	0.52
1:A:620:GLY:O	1:A:621:ILE:O	2.27	0.52
1:A:467:GLY:O	1:A:468:GLN:HB2	2.10	0.51
1:A:256:ILE:HG22	1:A:256:ILE:O	2.10	0.51
1:A:294:TYR:CE1	1:A:312:ASP:HB3	2.45	0.51
1:A:400:LEU:O	1:A:402:LEU:HD13	2.11	0.50
1:A:505:HIS:HB2	1:A:528:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:PRO:O	1:B:186:SER:HB2	2.12	0.50
1:A:282:HIS:CE1	1:A:367:ALA:HB1	2.46	0.49
1:A:271:HIS:O	1:A:278:ILE:HG21	2.12	0.49
1:B:256:ILE:HG22	1:B:256:ILE:O	2.11	0.49
1:A:280:ARG:HA	1:A:410:VAL:HG13	1.93	0.49
1:B:258:MET:HE3	1:B:261:GLY:O	2.12	0.49
1:B:341:LEU:HB3	1:B:364:GLN:HG2	1.95	0.48
1:A:341:LEU:HB3	1:A:364:GLN:HG2	1.94	0.48
1:B:280:ARG:HA	1:B:410:VAL:HG13	1.95	0.48
1:A:103:ALA:HB1	1:A:476:TYR:CD1	2.49	0.48
1:A:336:ASN:O	1:A:337:ASP:C	2.53	0.47
1:B:265:MET:HE2	1:B:295:LEU:HG	1.95	0.47
1:B:31:ILE:O	1:B:35:ILE:HG13	2.14	0.47
1:B:187:LYS:O	1:B:191:ILE:HG12	2.15	0.47
1:A:386:ASP:OD1	1:A:401:ARG:NE	2.43	0.47
1:B:400:LEU:O	1:B:402:LEU:HD13	2.15	0.47
1:A:187:LYS:O	1:A:191:ILE:HG12	2.15	0.47
1:B:468:GLN:H	1:B:494:HIS:CD2	2.32	0.47
1:B:336:ASN:O	1:B:337:ASP:C	2.53	0.47
1:B:158:MET:HG3	1:B:166:CYS:HB2	1.97	0.46
1:A:468:GLN:H	1:A:494:HIS:HD2	1.63	0.46
1:B:372:ALA:O	1:B:373:THR:HB	2.15	0.46
1:A:468:GLN:H	1:A:494:HIS:CD2	2.35	0.45
1:B:65:CYS:HB3	1:B:101:ILE:O	2.16	0.45
1:B:258:MET:HE2	1:B:261:GLY:O	2.17	0.45
1:A:358:ALA:HB3	1:A:360:PHE:HE1	1.82	0.45
1:A:329:LEU:HD23	1:A:360:PHE:CE2	2.52	0.44
1:A:8:SER:HB3	1:A:11:GLN:HB2	2.00	0.44
1:A:31:ILE:O	1:A:35:ILE:HG13	2.17	0.44
1:B:236:ASN:HB3	1:B:357:ASN:HD21	1.83	0.44
1:B:260:ASN:OD1	1:B:260:ASN:N	2.50	0.44
1:A:260:ASN:N	1:A:260:ASN:OD1	2.50	0.43
1:B:329:LEU:HD23	1:B:360:PHE:CE2	2.53	0.43
1:B:141:PHE:C	1:B:141:PHE:CD1	2.91	0.43
1:B:346:ILE:HD11	1:B:356:SER:HB3	2.00	0.43
1:B:272:PHE:O	1:B:303:VAL:HG22	2.19	0.43
1:A:346:ILE:HD11	1:A:356:SER:HB3	1.99	0.42
1:A:314:PHE:CD1	1:A:314:PHE:C	2.93	0.42
1:B:103:ALA:HB1	1:B:476:TYR:CD1	2.54	0.42
1:B:195:PHE:N	1:B:196:PRO:CD	2.83	0.42
1:A:99:ASN:HA	1:A:146:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ALA:HB3	1:B:360:PHE:HE1	1.84	0.42
1:B:280:ARG:O	1:B:409:TYR:HA	2.20	0.42
1:A:427:PRO:HD2	1:A:577:HIS:CD2	2.56	0.41
1:A:223:ASP:CG	1:A:224:THR:H	2.24	0.41
1:A:141:PHE:CD1	1:A:141:PHE:C	2.93	0.41
1:A:554:LEU:HG	1:A:587:ILE:HD11	2.01	0.41
1:A:539:GLU:HB2	1:A:542:GLU:HG3	2.02	0.41
1:A:39:PHE:O	1:A:470:ILE:HB	2.20	0.41
1:A:65:CYS:HB3	1:A:101:ILE:O	2.21	0.41
1:A:531:VAL:HG12	1:A:584:ARG:CG	2.51	0.41
1:A:236:ASN:HB3	1:A:357:ASN:HD21	1.86	0.41
1:A:346:ILE:HD12	1:A:356:SER:HB3	2.03	0.41
1:A:381:TYR:HB3	1:A:400:LEU:HG	2.03	0.41
1:A:61:ILE:HG23	1:A:472:ILE:HG22	2.03	0.41
1:B:8:SER:HB3	1:B:11:GLN:HB2	2.02	0.41
1:A:616:ARG:HH12	1:A:621:ILE:HD12	1.86	0.40
1:B:99:ASN:HA	1:B:146:LEU:HD13	2.04	0.40
1:A:462:PHE:CD2	1:A:485:LEU:HD13	2.57	0.40
1:B:61:ILE:HG23	1:B:472:ILE:HG22	2.03	0.40
1:A:175:SER:N	1:A:176:PRO:CD	2.84	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	620/622 (100%)	593 (96%)	25 (4%)	2 (0%)	41 61
1	B	620/622 (100%)	588 (95%)	30 (5%)	2 (0%)	41 61
All	All	1240/1244 (100%)	1181 (95%)	55 (4%)	4 (0%)	41 61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	591	ASN
1	B	373	THR
1	B	337	ASP
1	A	337	ASP

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	551/551 (100%)	520 (94%)	31 (6%)	21	36
1	B	551/551 (100%)	518 (94%)	33 (6%)	19	33
All	All	1102/1102 (100%)	1038 (94%)	64 (6%)	20	35

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	LYS
1	A	14	LYS
1	A	43	GLU
1	A	82	SER
1	A	84	SER
1	A	96	ARG
1	A	132	GLU
1	A	158	MET
1	A	186	SER
1	A	189	SER
1	A	198	LYS
1	A	204	VAL
1	A	255	GLN
1	A	259	ARG
1	A	260	ASN
1	A	291	GLU
1	A	301	ASN
1	A	321	ASN
1	A	326	LEU

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Mol	Chain	Res	Type
1	A	410	VAL
1	A	425	GLU
1	A	426	THR
1	A	548	LEU
1	A	581	LEU
1	A	583	LEU
1	A	591	ASN
1	A	596	LEU
1	A	597	PHE
1	A	609	PHE
1	A	617	GLN
1	B	3	ARG
1	B	4	LYS
1	B	14	LYS
1	B	43	GLU
1	B	84	SER
1	B	96	ARG
1	B	132	GLU
1	B	147	PRO
1	B	154	ASN
1	B	158	MET
1	B	175	SER
1	B	186	SER
1	B	189	SER
1	B	198	LYS
1	B	204	VAL
1	B	255	GLN
1	B	259	ARG
1	B	260	ASN
1	B	301	ASN
1	B	320	SER
1	B	321	ASN
1	B	403	PRO
1	B	410	VAL
1	B	426	THR
1	B	548	LEU
1	B	581	LEU
1	B	583	LEU
1	B	589	GLU
1	B	596	LEU
1	B	597	PHE
1	B	609	PHE

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Mol	Chain	Res	Type
1	B	617	GLN
1	B	621	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	89	ASN
1	A	134	ASN
1	A	150	ASN
1	A	229	HIS
1	A	249	GLN
1	A	282	HIS
1	A	301	ASN
1	A	321	ASN
1	A	357	ASN
1	A	431	ASN
1	A	494	HIS
1	A	541	HIS
1	A	577	HIS
1	B	89	ASN
1	B	134	ASN
1	B	150	ASN
1	B	229	HIS
1	B	282	HIS
1	B	321	ASN
1	B	357	ASN
1	B	431	ASN
1	B	494	HIS
1	B	541	HIS
1	B	577	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	B	701	-	24,26,26	0.40	0	37,40,40	0.64	0
2	U2F	A	701	-	35,38,38	0.48	0	51,58,58	1.22	4 (7%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UDP	B	701	-	-	4/16/32/32	0/2/2/2
2	U2F	A	701	-	-	9/22/59/59	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	U2F	O3'-C3'-C2'	-4.54	97.14	111.82
2	A	701	U2F	PA-O3A-PB	-4.20	118.41	132.83
2	A	701	U2F	O3A-PB-O1	-2.74	96.97	102.48
2	A	701	U2F	O2A-PA-O1A	2.05	122.39	112.24

There are no chirality outliers.

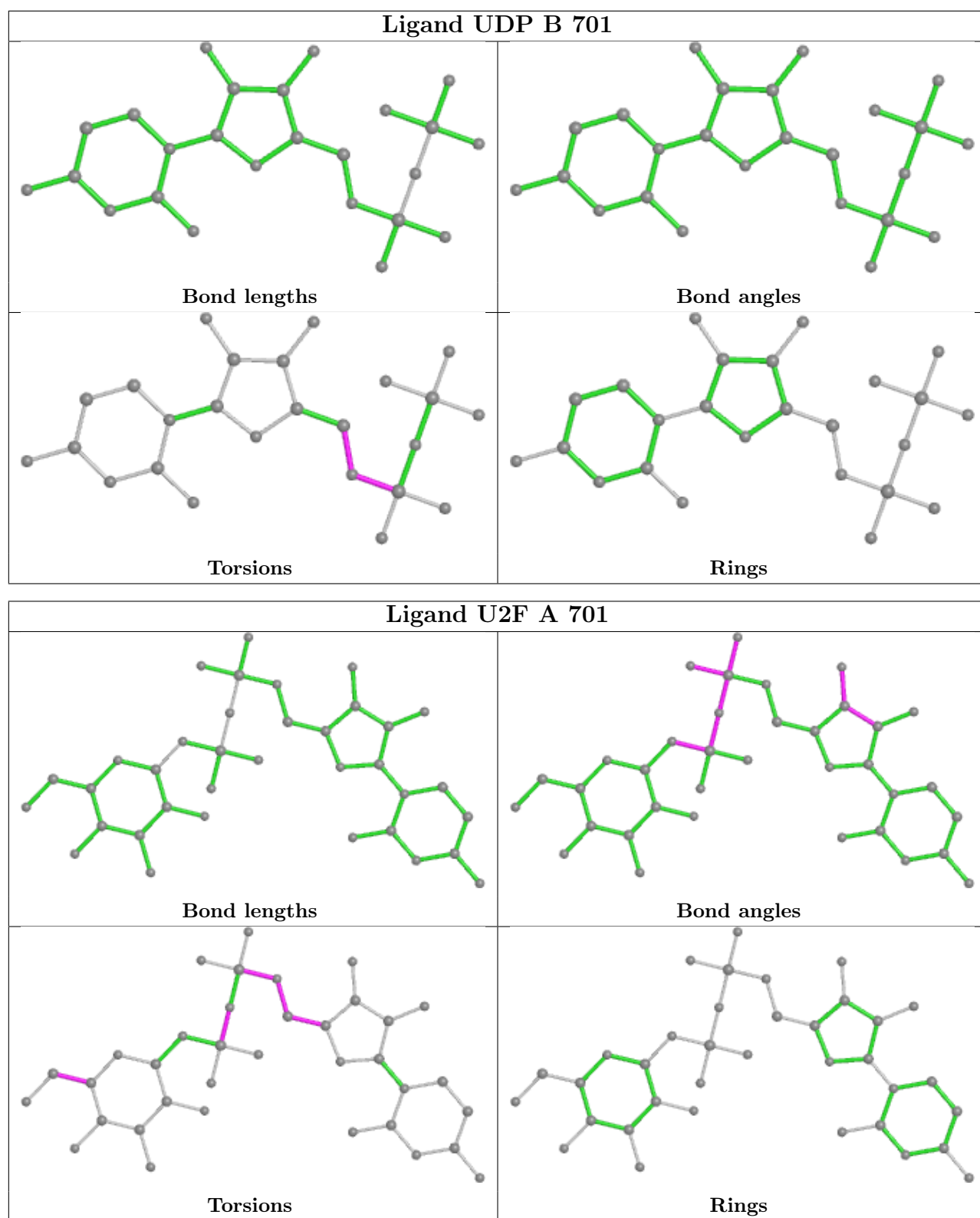
All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	U2F	C5'-O5'-PA-O2A
3	B	701	UDP	C5'-O5'-PA-O1A
2	A	701	U2F	O5-C5-C6-O6
2	A	701	U2F	O4'-C4'-C5'-O5'
2	A	701	U2F	C4-C5-C6-O6
2	A	701	U2F	C3'-C4'-C5'-O5'
2	A	701	U2F	PA-O3A-PB-O1B
3	B	701	UDP	C4'-C5'-O5'-PA
3	B	701	UDP	C5'-O5'-PA-O3A
2	A	701	U2F	C4'-C5'-O5'-PA
2	A	701	U2F	PA-O3A-PB-O2B
2	A	701	U2F	C5'-O5'-PA-O3A
3	B	701	UDP	C5'-O5'-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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

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	622/622 (100%)	-0.17	5 (0%) 86 89	65, 98, 137, 182	0
1	B	622/622 (100%)	0.10	24 (3%) 39 43	67, 117, 176, 217	0
All	All	1244/1244 (100%)	-0.03	29 (2%) 60 67	65, 105, 169, 217	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	414	LEU	4.6
1	B	365	VAL	4.5
1	B	608	LEU	4.1
1	B	342	TYR	3.9
1	B	296	ILE	3.9
1	B	268	VAL	3.8
1	B	318	ASP	3.7
1	B	353	ILE	3.6
1	B	295	LEU	3.5
1	B	435	ALA	3.5
1	B	141	PHE	3.2
1	B	366	ILE	3.0
1	B	528	LEU	2.9
1	A	504	LEU	2.6
1	A	465	ALA	2.5
1	B	158	MET	2.5
1	A	434	ILE	2.5
1	B	243	LEU	2.4
1	B	269	LEU	2.4
1	A	98	LEU	2.3
1	B	28	LEU	2.3
1	B	266	VAL	2.2
1	B	434	ILE	2.2
1	B	265	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	465	ALA	2.2
1	B	464	PHE	2.2
1	B	282	HIS	2.1
1	A	489	ALA	2.1
1	B	363	ILE	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](#)

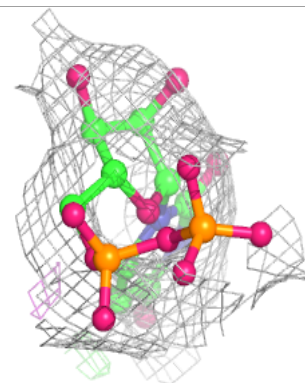
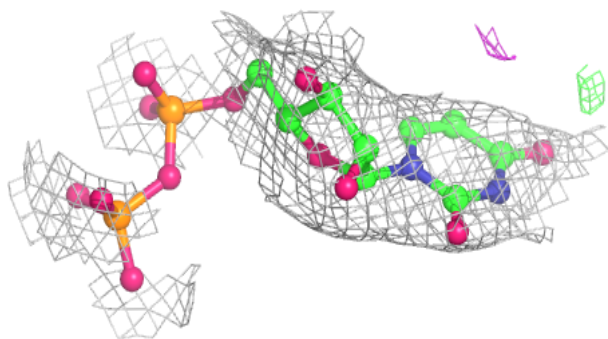
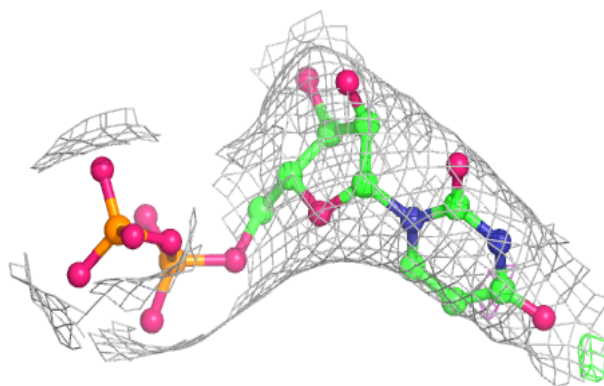
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UDP	B	701	25/25	0.85	0.15	119,131,191,195	0
2	U2F	A	701	36/36	0.93	0.13	88,117,163,172	0

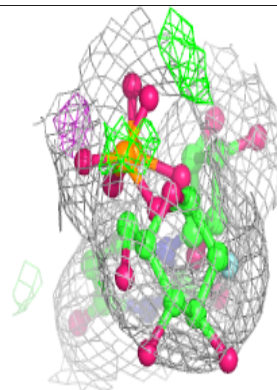
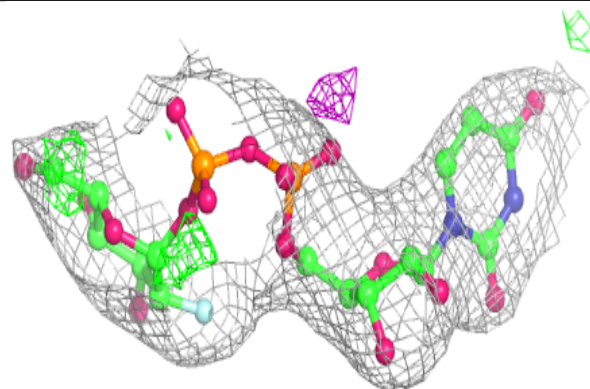
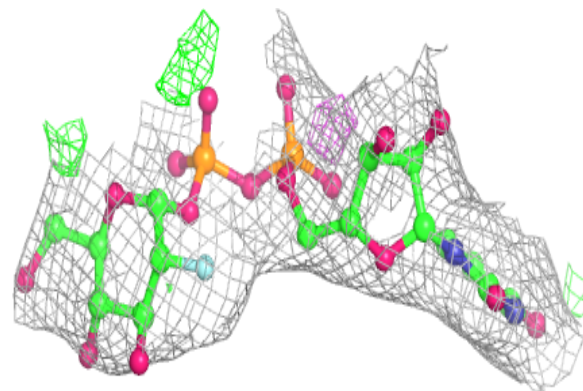
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UDP B 701:

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

**Electron density around U2F A 701:**

$2mF_o-DF_c$ (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.