



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 1, 2021 – 03:49 PM EDT

PDB ID : 2ZI6
Title : C4S dCK variant of dCK in complex with D-dA+UDP
Authors : Sabini, E.; Lavie, A.
Deposited on : 2008-02-13
Resolution : 1.77 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.23.2
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) : 2.23.2

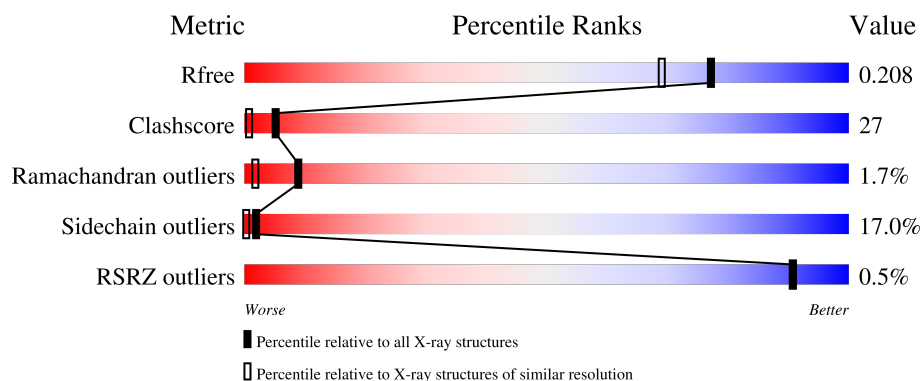
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	279	<div> <div></div> <div>33%</div> <div>36%</div> <div>8%</div> <div>•</div> <div>22%</div> </div>
1	B	279	<div> <div>39%</div> <div>32%</div> <div>9%</div> <div>19%</div> </div>
1	C	279	<div> <div>30%</div> <div>37%</div> <div>9%</div> <div>•</div> <div>23%</div> </div>
1	D	279	<div> <div>35%</div> <div>34%</div> <div>9%</div> <div>•</div> <div>22%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7616 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 Deoxycytidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	1	0
			1807	1165	299	337	6			
1	B	225	Total	C	N	O	S	0	1	0
			1867	1203	309	349	6			
1	C	216	Total	C	N	O	S	0	2	0
			1808	1167	300	335	6			
1	D	218	Total	C	N	O	S	0	0	0
			1797	1161	297	333	6			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	982	MET	-	expression tag	UNP P27707
A	983	GLY	-	expression tag	UNP P27707
A	984	SER	-	expression tag	UNP P27707
A	985	SER	-	expression tag	UNP P27707
A	986	HIS	-	expression tag	UNP P27707
A	987	HIS	-	expression tag	UNP P27707
A	988	HIS	-	expression tag	UNP P27707
A	989	HIS	-	expression tag	UNP P27707
A	990	HIS	-	expression tag	UNP P27707
A	991	HIS	-	expression tag	UNP P27707
A	992	SER	-	expression tag	UNP P27707
A	993	GLY	-	expression tag	UNP P27707
A	994	LEU	-	expression tag	UNP P27707
A	995	VAL	-	expression tag	UNP P27707
A	996	PRO	-	expression tag	UNP P27707
A	997	ARG	-	expression tag	UNP P27707
A	998	GLY	-	expression tag	UNP P27707
A	999	SER	-	expression tag	UNP P27707
A	1000	HIS	-	expression tag	UNP P27707
A	1009	SER	CYS	engineered mutation	UNP P27707
A	1045	SER	CYS	engineered mutation	UNP P27707

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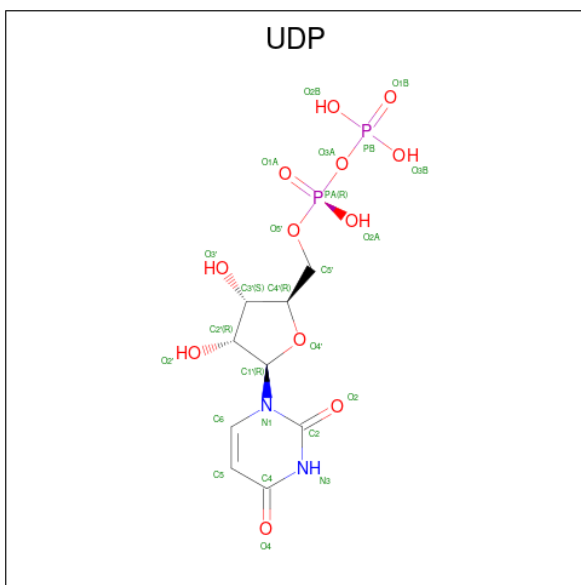
Chain	Residue	Modelled	Actual	Comment	Reference
A	1059	SER	CYS	engineered mutation	UNP P27707
A	1146	SER	CYS	engineered mutation	UNP P27707
B	1982	MET	-	expression tag	UNP P27707
B	1983	GLY	-	expression tag	UNP P27707
B	1984	SER	-	expression tag	UNP P27707
B	1985	SER	-	expression tag	UNP P27707
B	1986	HIS	-	expression tag	UNP P27707
B	1987	HIS	-	expression tag	UNP P27707
B	1988	HIS	-	expression tag	UNP P27707
B	1989	HIS	-	expression tag	UNP P27707
B	1990	HIS	-	expression tag	UNP P27707
B	1991	HIS	-	expression tag	UNP P27707
B	1992	SER	-	expression tag	UNP P27707
B	1993	GLY	-	expression tag	UNP P27707
B	1994	LEU	-	expression tag	UNP P27707
B	1995	VAL	-	expression tag	UNP P27707
B	1996	PRO	-	expression tag	UNP P27707
B	1997	ARG	-	expression tag	UNP P27707
B	1998	GLY	-	expression tag	UNP P27707
B	1999	SER	-	expression tag	UNP P27707
B	2000	HIS	-	expression tag	UNP P27707
B	2009	SER	CYS	engineered mutation	UNP P27707
B	2045	SER	CYS	engineered mutation	UNP P27707
B	2059	SER	CYS	engineered mutation	UNP P27707
B	2146	SER	CYS	engineered mutation	UNP P27707
C	2982	MET	-	expression tag	UNP P27707
C	2983	GLY	-	expression tag	UNP P27707
C	2984	SER	-	expression tag	UNP P27707
C	2985	SER	-	expression tag	UNP P27707
C	2986	HIS	-	expression tag	UNP P27707
C	2987	HIS	-	expression tag	UNP P27707
C	2988	HIS	-	expression tag	UNP P27707
C	2989	HIS	-	expression tag	UNP P27707
C	2990	HIS	-	expression tag	UNP P27707
C	2991	HIS	-	expression tag	UNP P27707
C	2992	SER	-	expression tag	UNP P27707
C	2993	GLY	-	expression tag	UNP P27707
C	2994	LEU	-	expression tag	UNP P27707
C	2995	VAL	-	expression tag	UNP P27707
C	2996	PRO	-	expression tag	UNP P27707
C	2997	ARG	-	expression tag	UNP P27707
C	2998	GLY	-	expression tag	UNP P27707

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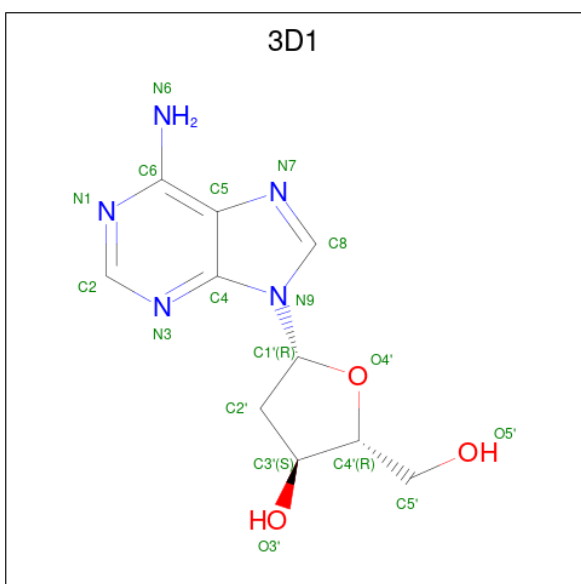
Chain	Residue	Modelled	Actual	Comment	Reference
C	2999	SER	-	expression tag	UNP P27707
C	3000	HIS	-	expression tag	UNP P27707
C	3009	SER	CYS	engineered mutation	UNP P27707
C	3045	SER	CYS	engineered mutation	UNP P27707
C	3059	SER	CYS	engineered mutation	UNP P27707
C	3146	SER	CYS	engineered mutation	UNP P27707
D	3982	MET	-	expression tag	UNP P27707
D	3983	GLY	-	expression tag	UNP P27707
D	3984	SER	-	expression tag	UNP P27707
D	3985	SER	-	expression tag	UNP P27707
D	3986	HIS	-	expression tag	UNP P27707
D	3987	HIS	-	expression tag	UNP P27707
D	3988	HIS	-	expression tag	UNP P27707
D	3989	HIS	-	expression tag	UNP P27707
D	3990	HIS	-	expression tag	UNP P27707
D	3991	HIS	-	expression tag	UNP P27707
D	3992	SER	-	expression tag	UNP P27707
D	3993	GLY	-	expression tag	UNP P27707
D	3994	LEU	-	expression tag	UNP P27707
D	3995	VAL	-	expression tag	UNP P27707
D	3996	PRO	-	expression tag	UNP P27707
D	3997	ARG	-	expression tag	UNP P27707
D	3998	GLY	-	expression tag	UNP P27707
D	3999	SER	-	expression tag	UNP P27707
D	4000	HIS	-	expression tag	UNP P27707
D	4009	SER	CYS	engineered mutation	UNP P27707
D	4045	SER	CYS	engineered mutation	UNP P27707
D	4059	SER	CYS	engineered mutation	UNP P27707
D	4146	SER	CYS	engineered mutation	UNP P27707

- 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		
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is (2R,3S,5R)-5-(6-amino-9H-purin-9-yl)-tetrahydro-2-(hydroxymethyl)furan-3-ol (three-letter code: 3D1) (formula: C₁₀H₁₃N₅O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	10	5	3		
3	B	1	Total	C	N	O	0	0
			18	10	5	3		
3	C	1	Total	C	N	O	0	0
			18	10	5	3		
3	D	1	Total	C	N	O	0	0
			18	10	5	3		

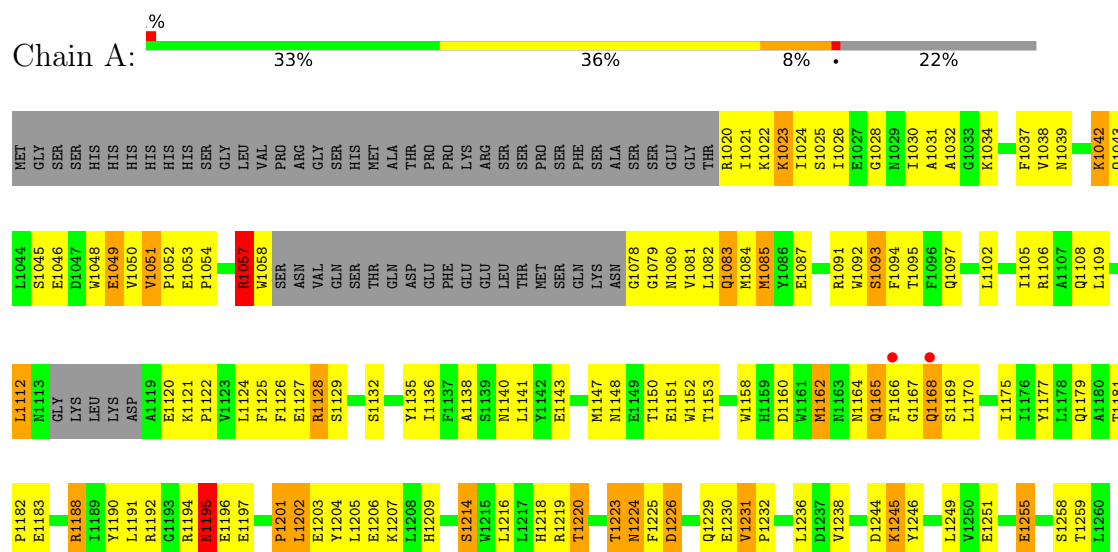
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	42	Total	O	0	0
			42	42		
4	C	38	Total	O	0	0
			38	38		
4	D	35	Total	O	0	0
			35	35		

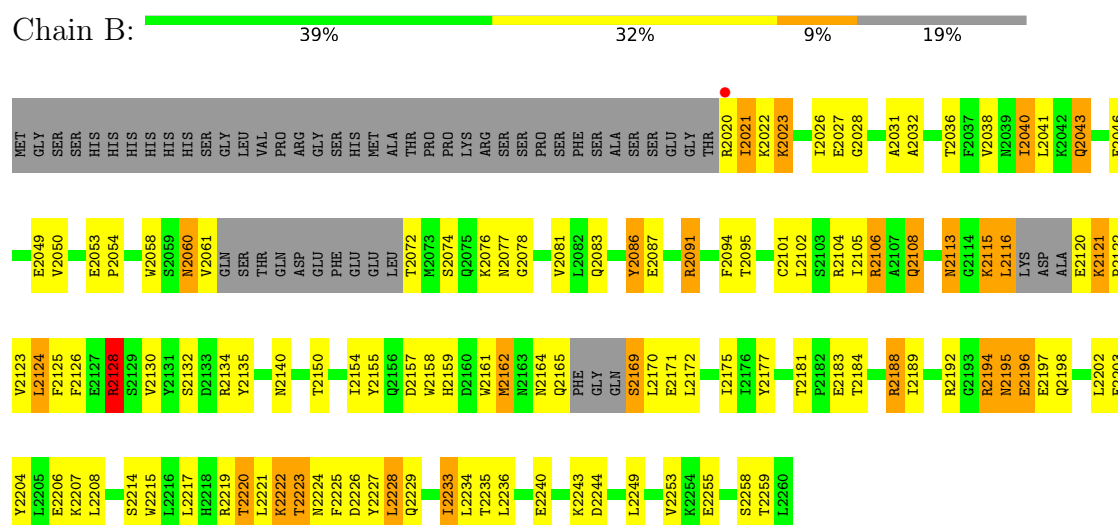
3 Residue-property plots

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: Deoxycytidine kinase

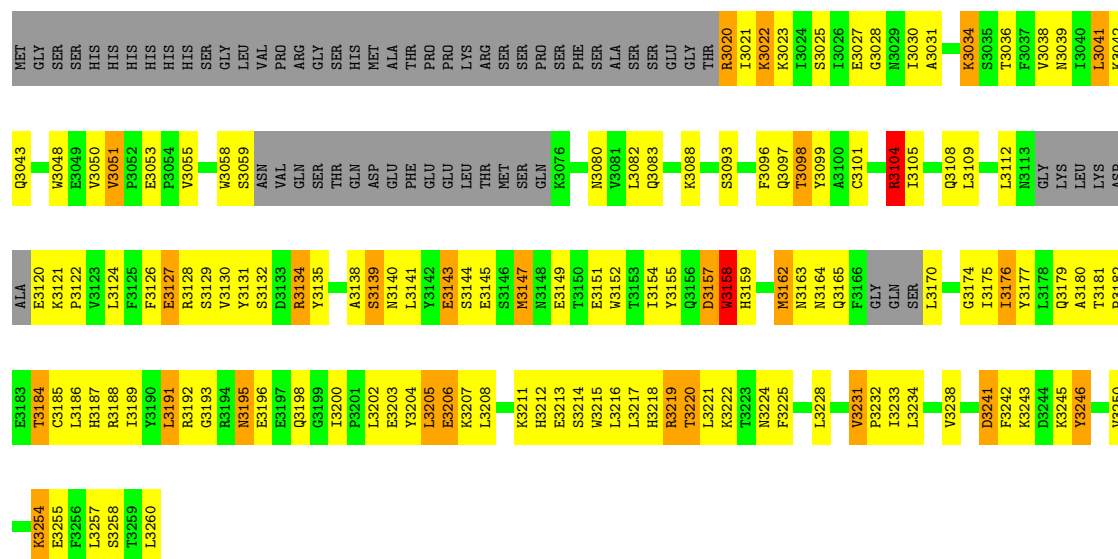


• Molecule 1: Deoxycytidine kinase



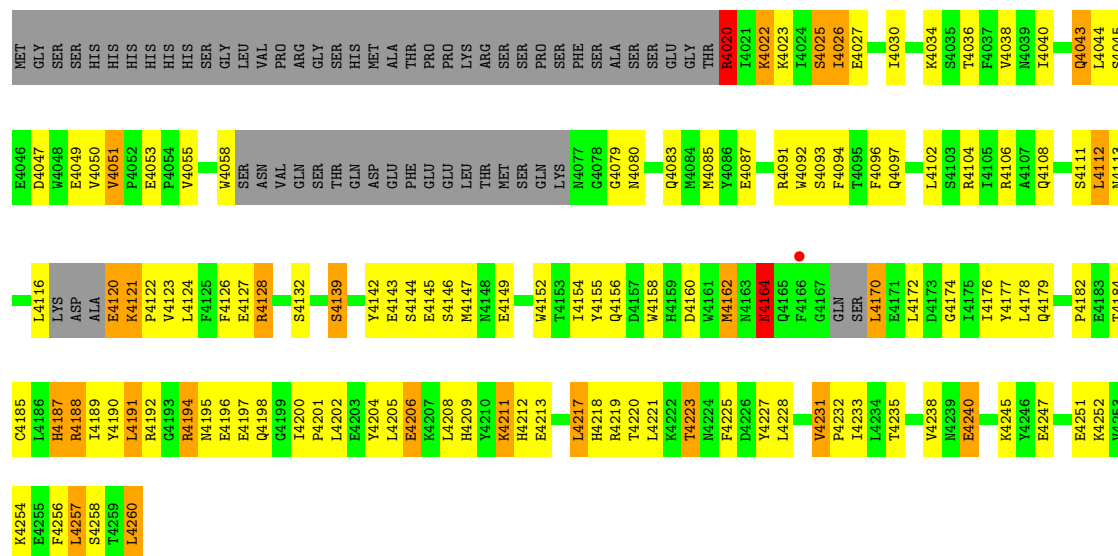
• Molecule 1: Deoxycytidine kinase





• Molecule 1: Deoxycytidine kinase

Chain D: 35% 34% 9% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	138.25Å 138.51Å 118.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.77 29.96 – 1.77	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.77) 97.4 (29.96-1.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 1.77Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.208 , 0.283 0.209 , 0.208	Depositor DCC
R_{free} test set	11026 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.468 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7616	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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 62.04 % 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 1.1957e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3D1, 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	0.40	0/1855	1.25	11/2513 (0.4%)
1	B	0.41	0/1913	1.35	13/2590 (0.5%)
1	C	0.40	0/1854	1.30	14/2509 (0.6%)
1	D	0.40	0/1840	1.30	15/2492 (0.6%)
All	All	0.40	0/7462	1.30	53/10104 (0.5%)

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2091	ARG	NE-CZ-NH1	-15.12	112.74	120.30
1	C	3104	ARG	NE-CZ-NH1	-12.06	114.27	120.30
1	B	2091	ARG	NE-CZ-NH2	9.53	125.07	120.30
1	D	4020	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	D	4020	ARG	CD-NE-CZ	8.91	136.08	123.60

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	1807	0	1739	113	0
1	B	1867	0	1819	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1808	0	1752	92	0
1	D	1797	0	1731	97	0
2	A	100	0	44	9	0
3	A	18	0	13	1	0
3	B	18	0	13	0	0
3	C	18	0	13	1	0
3	D	18	0	13	0	0
4	A	50	0	0	1	0
4	B	42	0	0	3	0
4	C	38	0	0	1	0
4	D	35	0	0	1	0
All	All	7616	0	7137	391	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 27.

The worst 5 of 391 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:1023:LYS:HD3	1:A:1169:SER:O	1.53	1.08
1:A:1023:LYS:CD	1:A:1169:SER:O	2.09	1.00
1:A:1166:PHE:HA	1:A:1168:GLN:HG2	1.54	0.88
1:A:1051:VAL:HG21	1:A:1108:GLN:HG2	1.55	0.86
1:D:4123:VAL:HG21	1:D:4257:LEU:HD11	1.59	0.85

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	212/279 (76%)	193 (91%)	13 (6%)	6 (3%)	5 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	218/279 (78%)	195 (89%)	19 (9%)	4 (2%)	8	1
1	C	210/279 (75%)	185 (88%)	23 (11%)	2 (1%)	15	4
1	D	210/279 (75%)	191 (91%)	17 (8%)	2 (1%)	15	4
All	All	850/1116 (76%)	764 (90%)	72 (8%)	14 (2%)	9	2

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1168	GLN
1	A	1195	ASN
1	B	2113	ASN
1	B	2195	ASN
1	B	2226	ASP

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	195/255 (76%)	168 (86%)	27 (14%)	3	0
1	B	205/255 (80%)	171 (83%)	34 (17%)	2	0
1	C	197/255 (77%)	158 (80%)	39 (20%)	1	0
1	D	193/255 (76%)	158 (82%)	35 (18%)	1	0
All	All	790/1020 (78%)	655 (83%)	135 (17%)	2	0

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4139	SER
1	D	4149	GLU
1	D	4240	GLU
1	B	2195	ASN
1	B	2172	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3218	HIS
1	D	4043	GLN
1	D	4195	ASN
1	D	4164	ASN
1	D	4039	ASN

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 ⓘ

8 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	$\# Z > 2$
2	UDP	A	2301	-	20,26,26	1.21	2 (10%)	25,40,40	1.03	0
3	3D1	C	3302	-	18,20,20	2.21	2 (11%)	17,29,29	3.09	5 (29%)
3	3D1	D	4302	-	18,20,20	2.31	2 (11%)	17,29,29	3.13	7 (41%)
2	UDP	A	4301	-	20,26,26	1.40	3 (15%)	25,40,40	1.20	4 (16%)
3	3D1	A	1302	-	18,20,20	2.23	3 (16%)	17,29,29	3.02	5 (29%)
2	UDP	A	3301	-	20,26,26	1.24	1 (5%)	25,40,40	1.29	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	3D1	B	2302	-	18,20,20	2.22	3 (16%)	17,29,29	2.97	5 (29%)
2	UDP	A	1301	-	20,26,26	1.42	3 (15%)	25,40,40	1.32	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDP	A	2301	-	-	4/14/32/32	0/2/2/2
3	3D1	C	3302	-	-	0/2/18/18	0/3/3/3
3	3D1	D	4302	-	-	0/2/18/18	0/3/3/3
2	UDP	A	4301	-	-	0/14/32/32	0/2/2/2
3	3D1	A	1302	-	-	0/2/18/18	0/3/3/3
2	UDP	A	3301	-	-	3/14/32/32	0/2/2/2
3	3D1	B	2302	-	-	0/2/18/18	0/3/3/3
2	UDP	A	1301	-	-	3/14/32/32	0/2/2/2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4302	3D1	C2-N3	7.64	1.44	1.32
3	B	2302	3D1	C2-N3	7.50	1.44	1.32
3	C	3302	3D1	C2-N3	7.27	1.43	1.32
3	A	1302	3D1	C2-N3	7.22	1.43	1.32
3	D	4302	3D1	C2-N1	4.64	1.42	1.33

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3302	3D1	N3-C2-N1	-9.51	113.82	128.68
3	D	4302	3D1	N3-C2-N1	-9.23	114.26	128.68
3	A	1302	3D1	N3-C2-N1	-9.20	114.29	128.68
3	B	2302	3D1	N3-C2-N1	-8.75	115.00	128.68
3	B	2302	3D1	C2-N1-C6	6.17	129.31	118.75

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	UDP	O4'-C1'-N1-C6
2	A	1301	UDP	PA-O3A-PB-O3B
2	A	2301	UDP	C2'-C1'-N1-C6
2	A	2301	UDP	O4'-C1'-N1-C6
2	A	2301	UDP	PA-O3A-PB-O3B

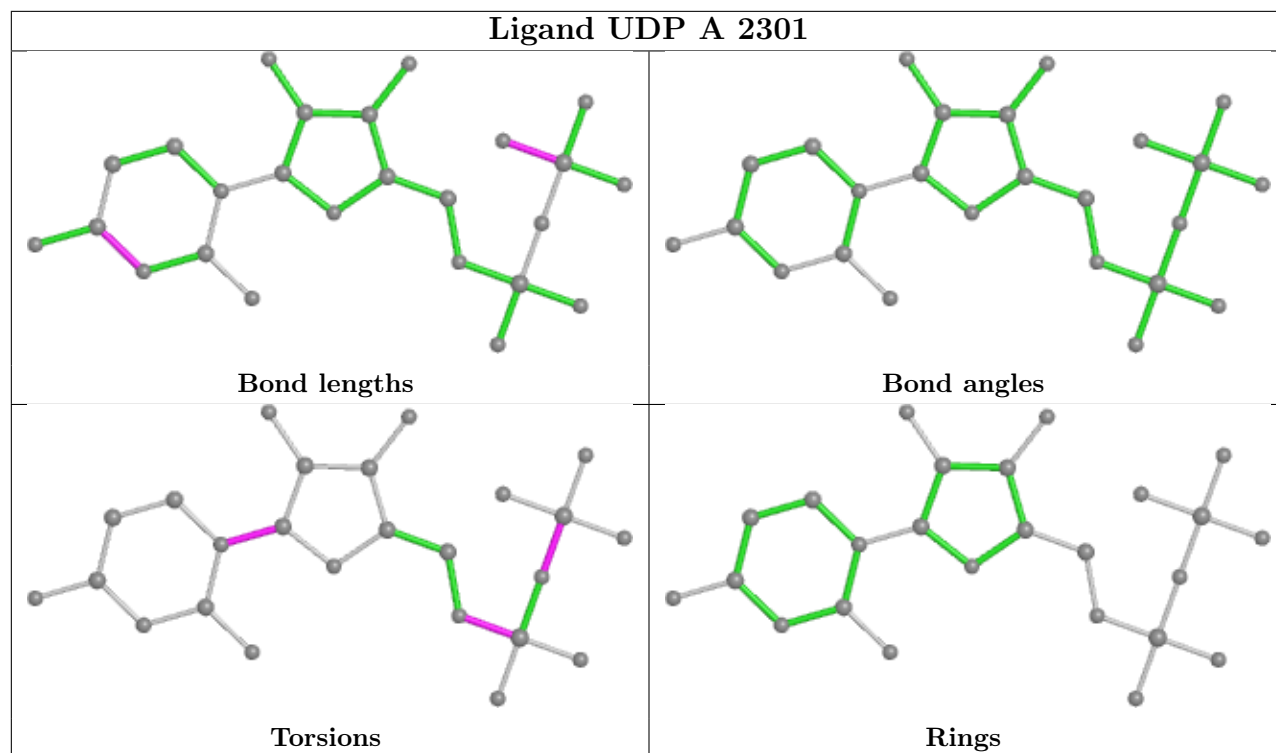
There are no ring outliers.

6 monomers are involved in 11 short contacts:

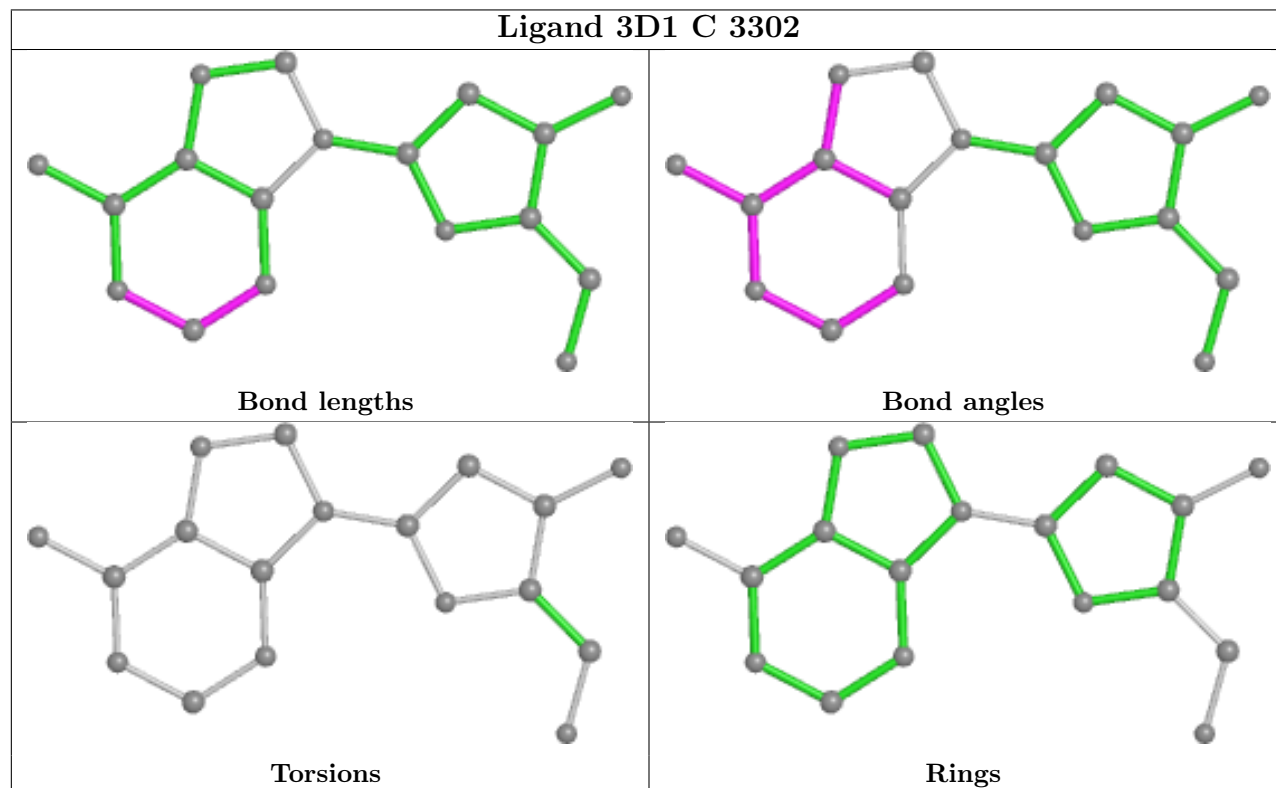
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2301	UDP	2	0
3	C	3302	3D1	1	0
2	A	4301	UDP	1	0
3	A	1302	3D1	1	0
2	A	3301	UDP	3	0
2	A	1301	UDP	3	0

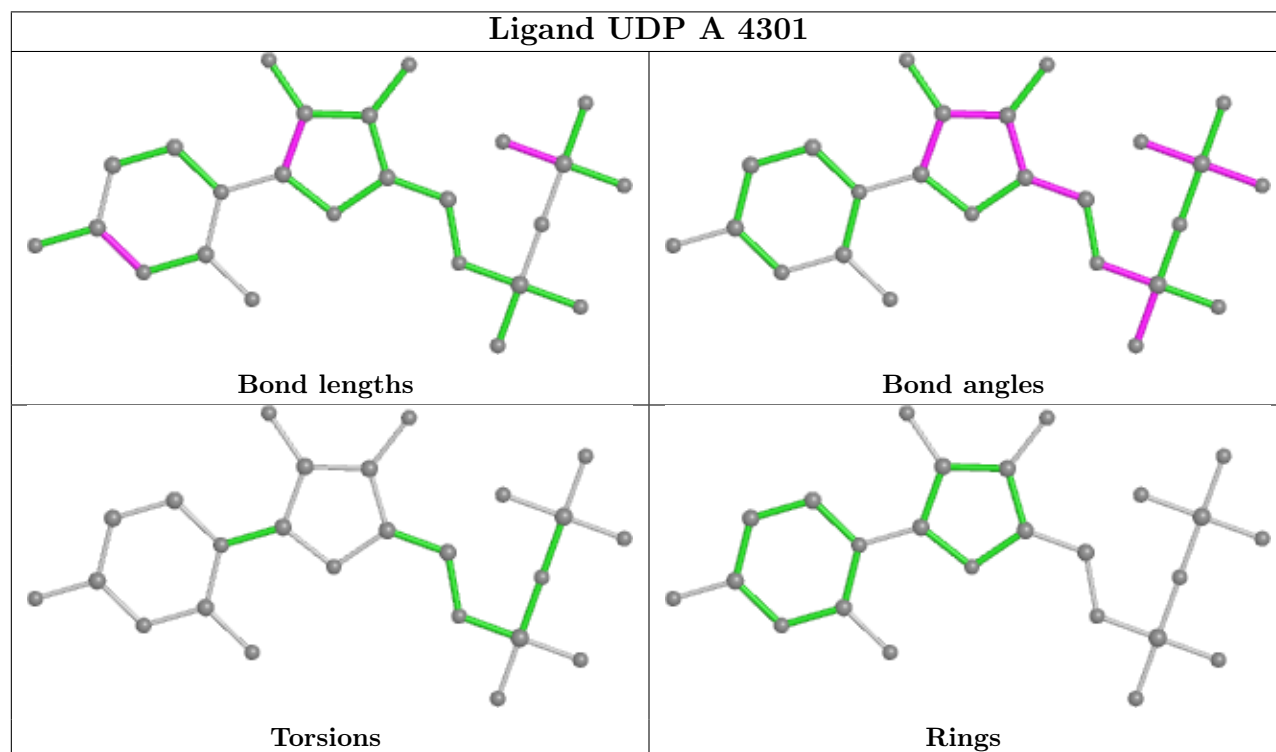
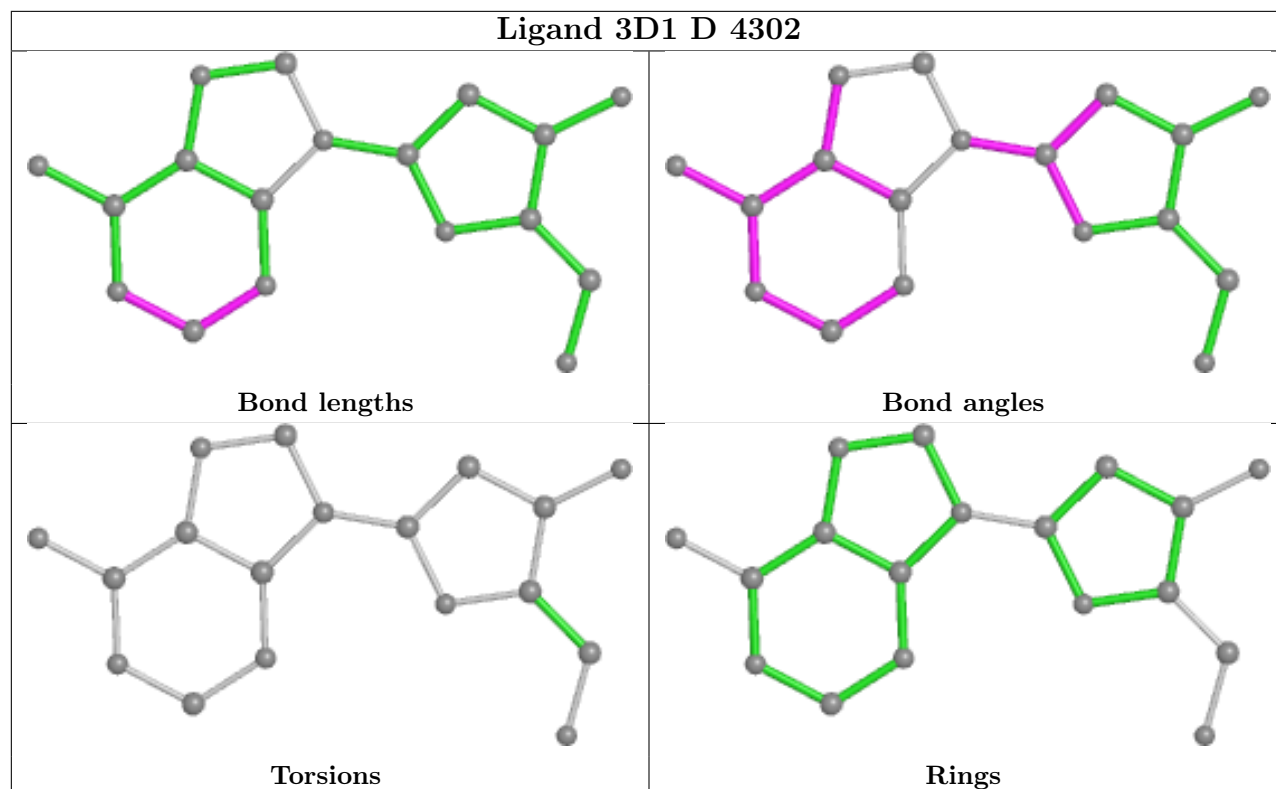
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

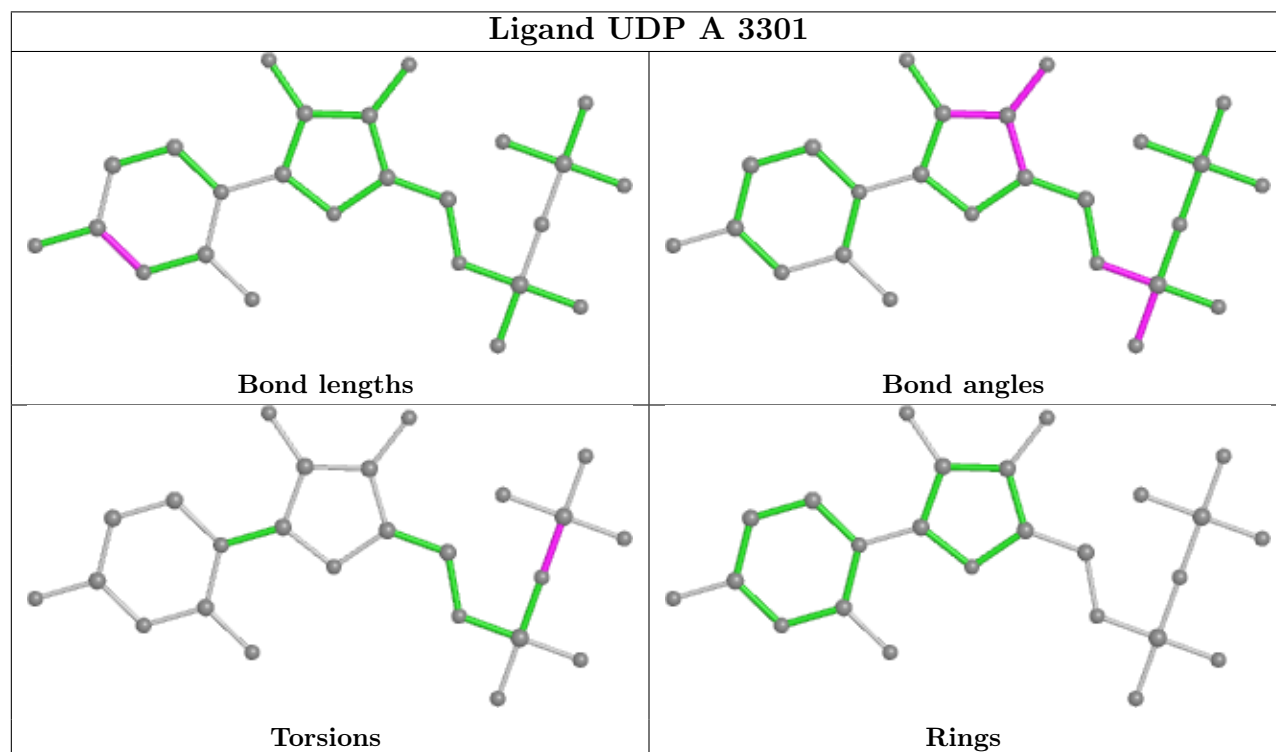
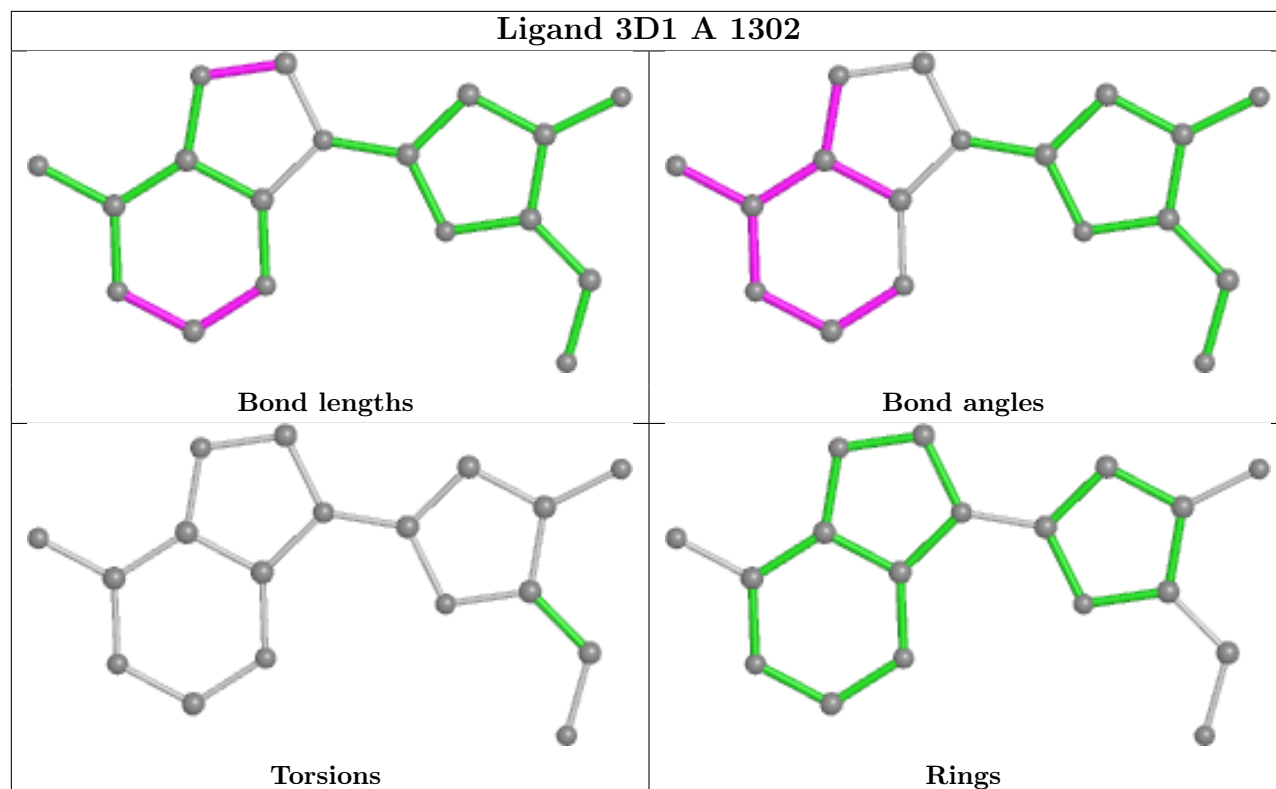
Ligand UDP A 2301

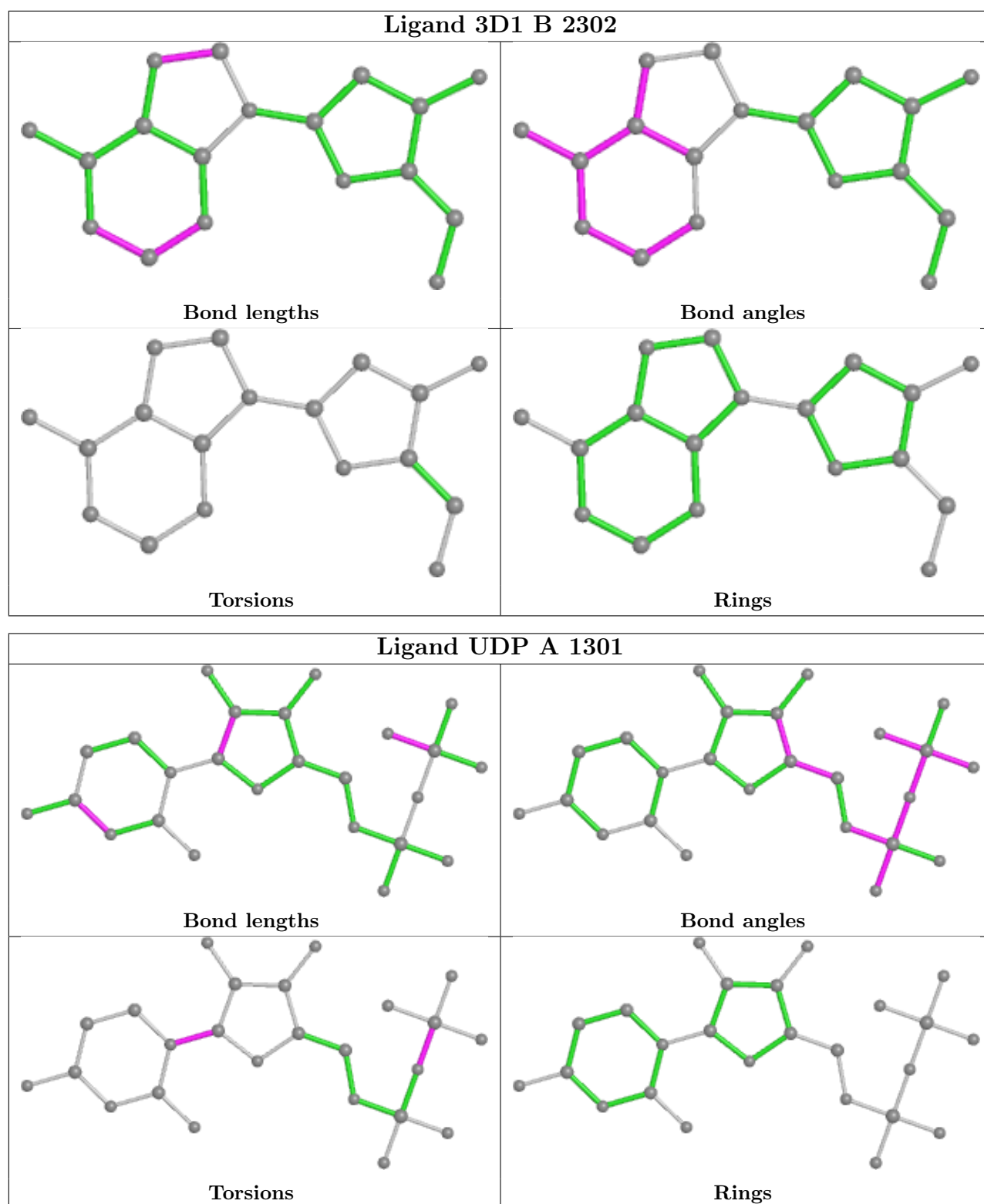


Ligand 3D1 C 3302









5.7 Other polymers ⓘ

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 [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	217/279 (77%)	-0.14	2 (0%) 84 84	14, 28, 46, 62	0
1	B	225/279 (80%)	-0.24	1 (0%) 92 92	11, 24, 41, 60	0
1	C	216/279 (77%)	-0.21	0 100 100	13, 29, 47, 56	0
1	D	218/279 (78%)	-0.25	1 (0%) 91 91	13, 25, 44, 61	0
All	All	876/1116 (78%)	-0.21	4 (0%) 91 91	11, 27, 46, 62	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1166	PHE	2.5
1	D	4166	PHE	2.5
1	B	2020	ARG	2.3
1	A	1168	GLN	2.2

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](#)

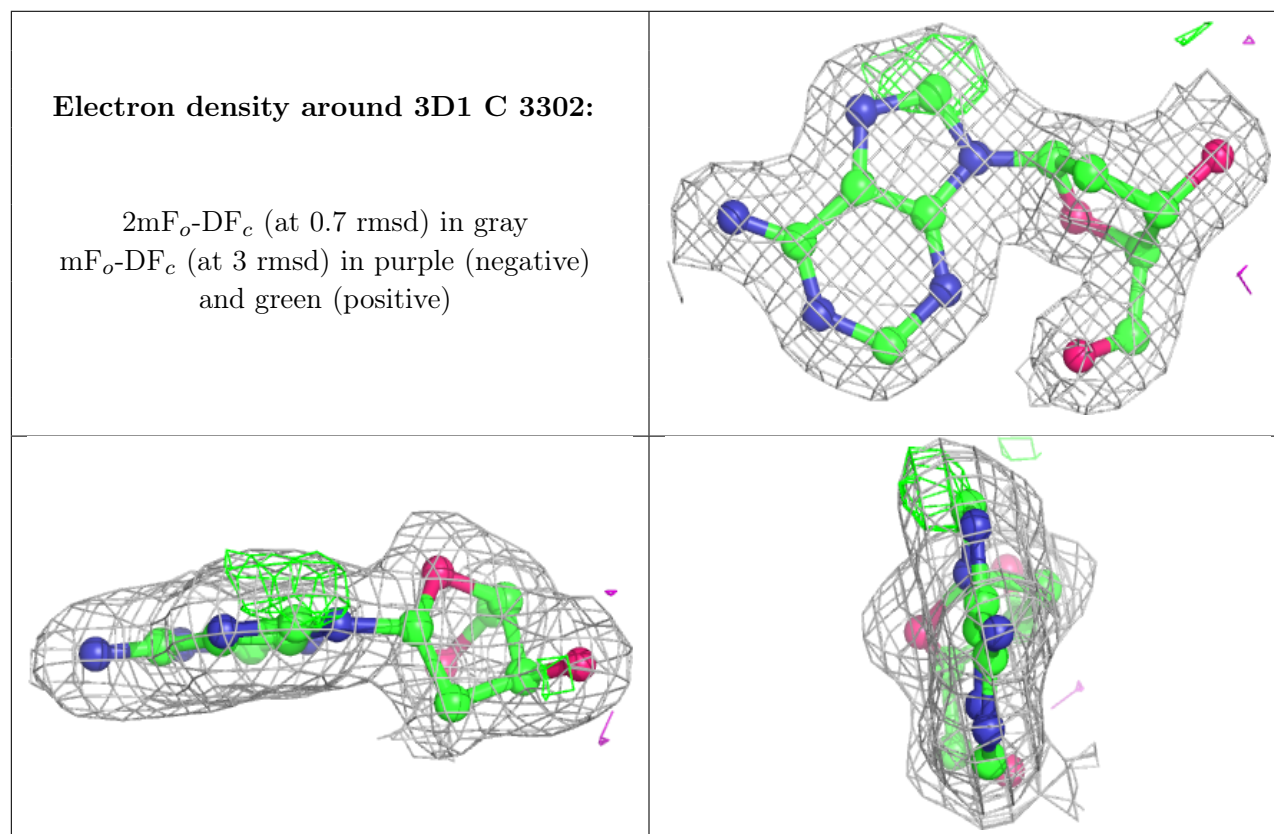
There are no monosaccharides in this entry.

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.

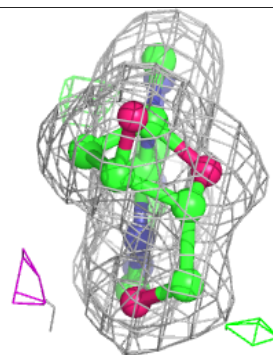
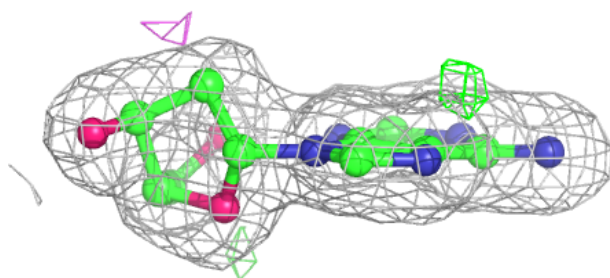
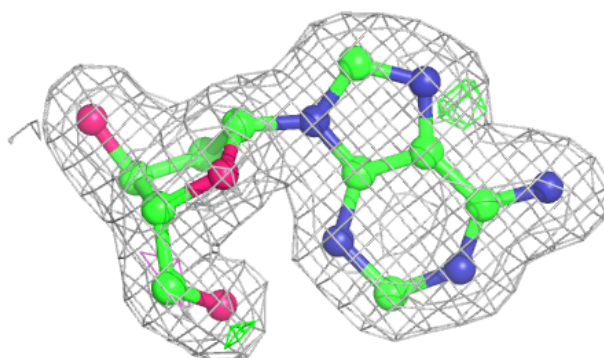
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	3D1	C	3302	18/18	0.92	0.09	26,29,33,34	0
3	3D1	B	2302	18/18	0.96	0.08	15,17,20,24	0
3	3D1	A	1302	18/18	0.97	0.07	11,23,27,27	0
2	UDP	A	1301	25/25	0.98	0.08	4,25,33,36	0
2	UDP	A	2301	25/25	0.98	0.08	9,23,28,39	0
2	UDP	A	3301	25/25	0.98	0.07	13,24,33,33	0
3	3D1	D	4302	18/18	0.98	0.07	13,20,21,22	0
2	UDP	A	4301	25/25	0.99	0.07	17,22,28,33	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.

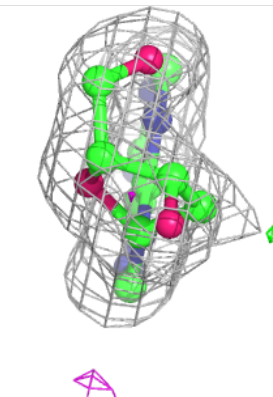
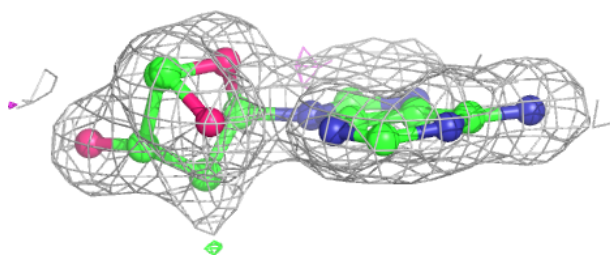
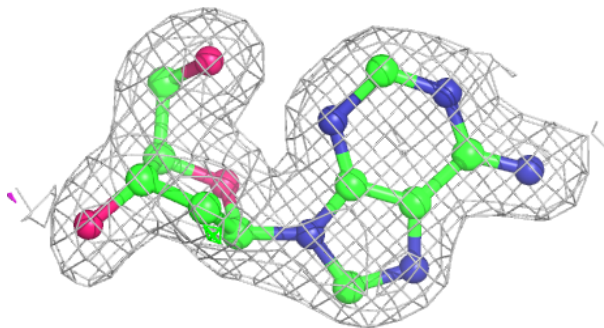


Electron density around 3D1 B 2302:

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

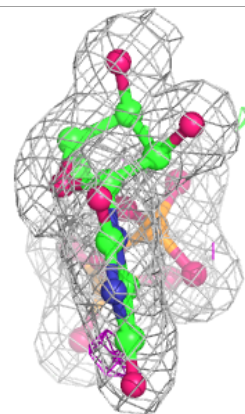
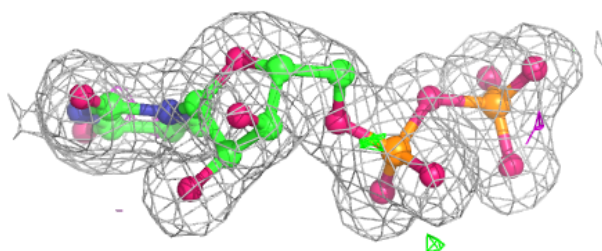
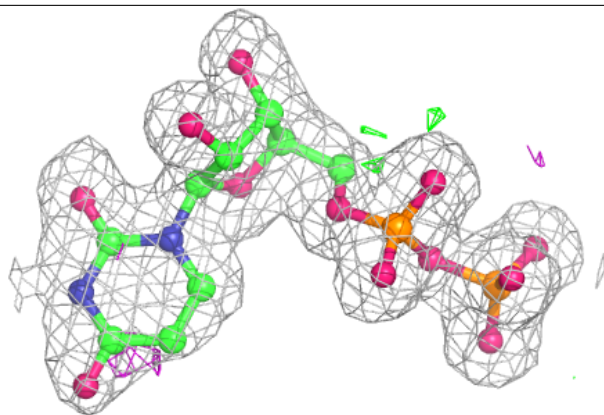
**Electron density around 3D1 A 1302:**

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

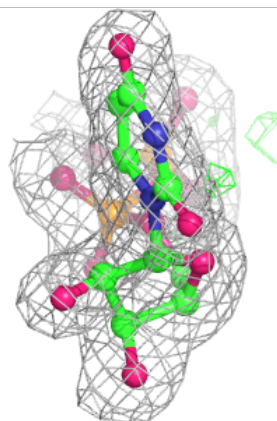
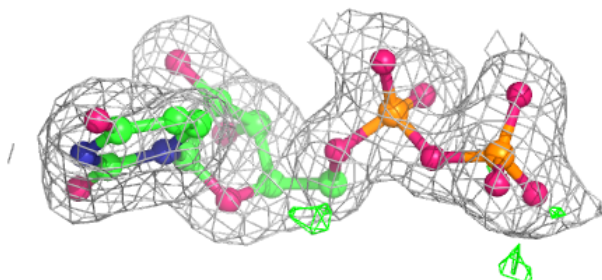
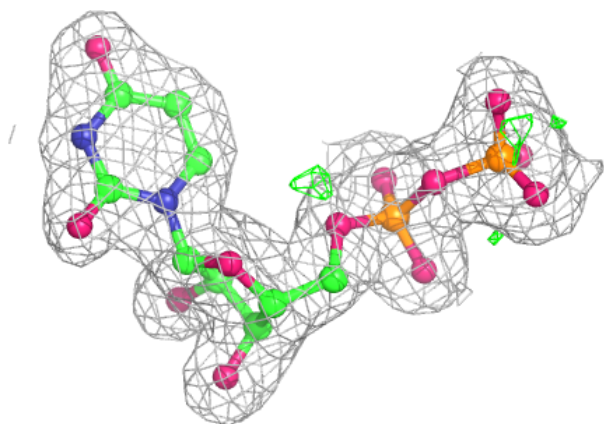


Electron density around UDP A 1301:

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

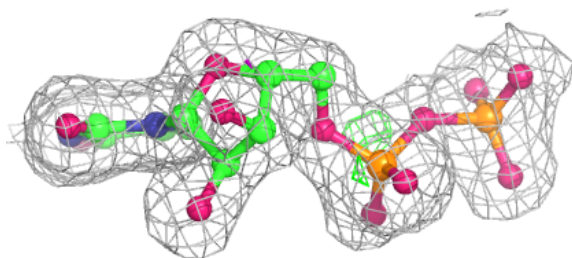
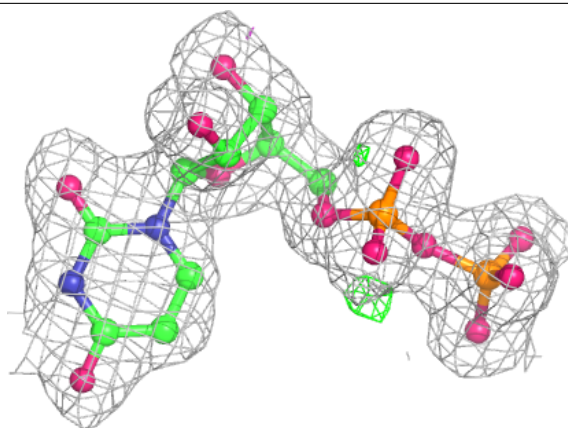
**Electron density around UDP A 2301:**

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

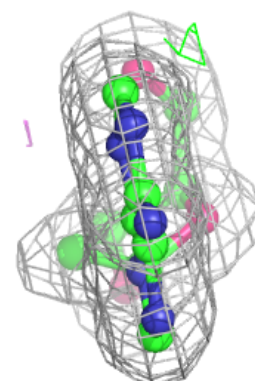
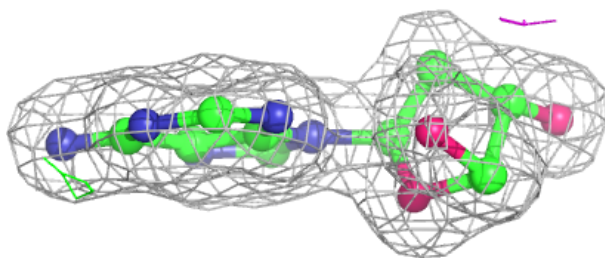
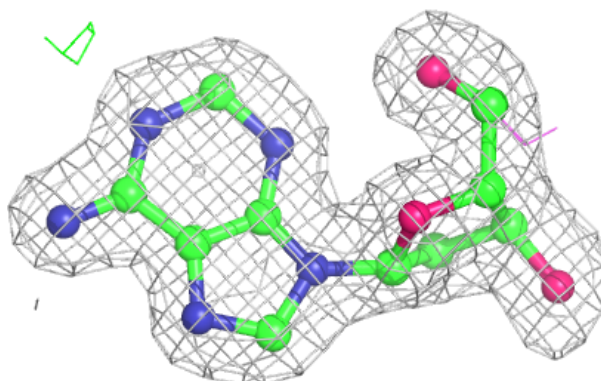


Electron density around UDP A 3301:

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

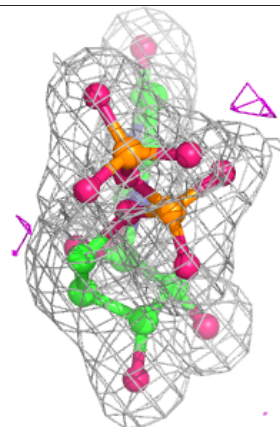
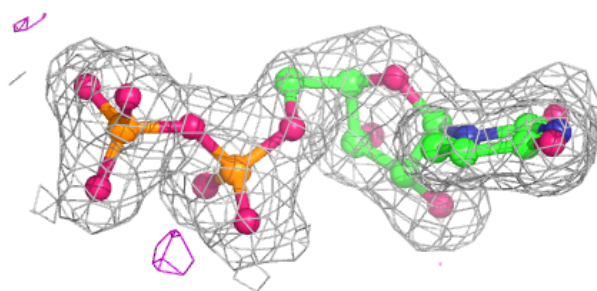
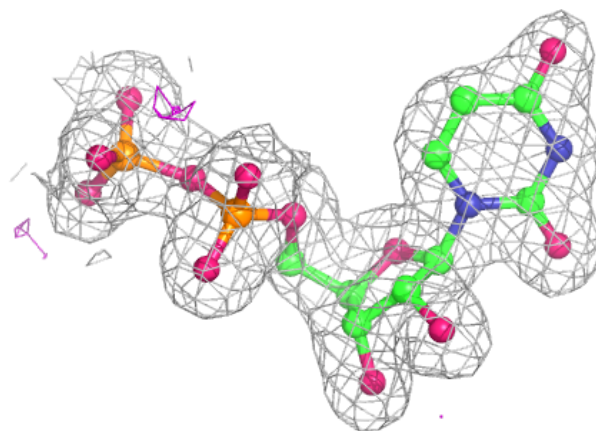
**Electron density around 3D1 D 4302:**

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



Electron density around UDP A 4301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.