Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 04:18 AM EDT

PDB ID	:	7L7Y
Title	:	x-ray structure of the N-acetyltransferase Pcryo_0637 from psychrobacter cryohalolentis in the presence of UDP and acetyl-conezyme A
Authors	:	Linehan, M.P.; Thoden, J.B.; Holden, H.M.
Deposited on	:	2020-12-30
Resolution	:	1.30 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:

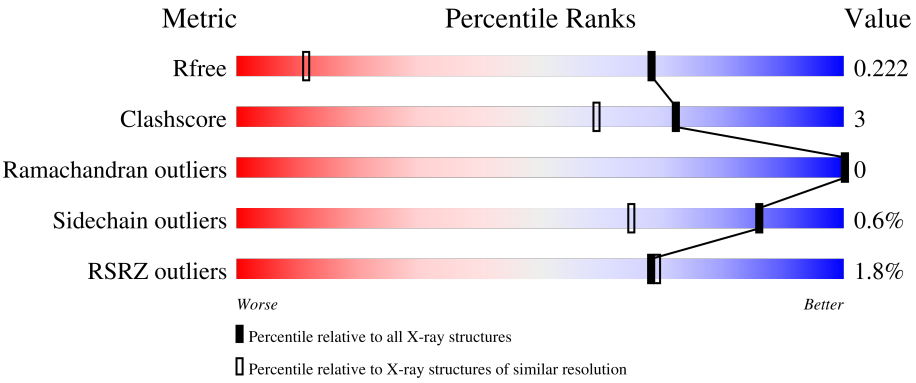
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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	AAA	227	2% 88% 7% .

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 2006 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.

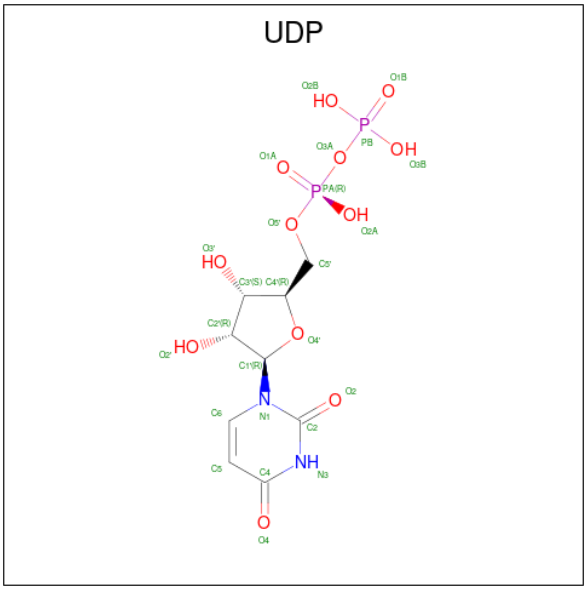
- Molecule 1 is a protein called Putative acetyl transferase protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	217	1642	1051	272	309	10	0	5	0

There are 8 discrepancies between the modelled and reference sequences:

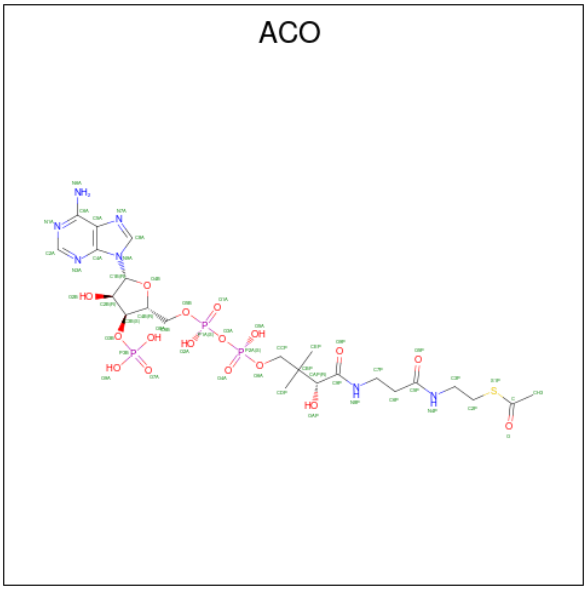
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	220	LEU	-	expression tag	UNP Q1QD33
AAA	221	GLU	-	expression tag	UNP Q1QD33
AAA	222	HIS	-	expression tag	UNP Q1QD33
AAA	223	HIS	-	expression tag	UNP Q1QD33
AAA	224	HIS	-	expression tag	UNP Q1QD33
AAA	225	HIS	-	expression tag	UNP Q1QD33
AAA	226	HIS	-	expression tag	UNP Q1QD33
AAA	227	HIS	-	expression tag	UNP Q1QD33

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



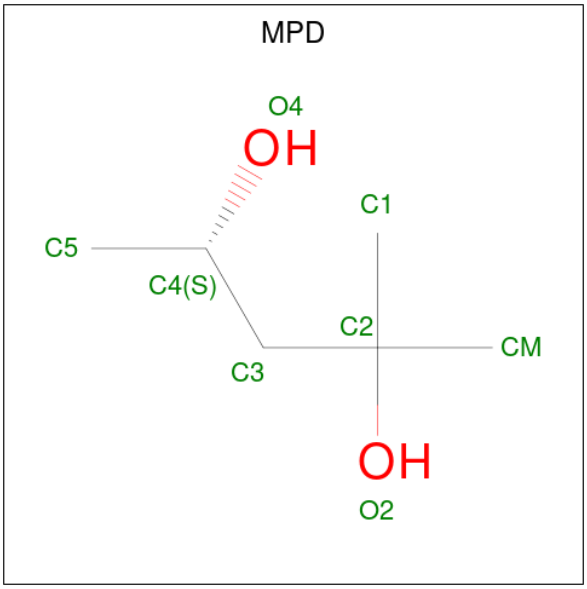
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	1
			50	18	4	24	4		

- Molecule 3 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 8 6 2	0	0
4	AAA	1	Total C O 8 6 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total Cl 1 1	0	0

- Molecule 6 is water.

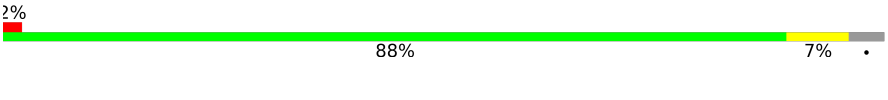
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	246	Total O 246 246	0	0

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: Putative acetyl transferase protein

Chain AAA:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	97.66Å 97.66Å 65.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.75 – 1.30 28.73 – 1.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.75-1.30) 98.3 (28.73-1.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.194 , 0.214 0.203 , 0.222	Depositor DCC
R_{free} test set	2917 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	6.0	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	2006	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACO, CL, MPD, 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	AAA	0.66	0/1687	0.80	0/2291

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

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	AAA	1642	0	1687	9	0
2	AAA	50	0	22	2	0
3	AAA	51	0	34	1	0
4	AAA	16	0	28	0	0
5	AAA	1	0	0	0	0
6	AAA	246	0	0	2	1
All	All	2006	0	1771	12	1

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 3.

All (12) 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)
2:AAA:301[B]:UDP:O1A	6:AAA:401:HOH:O	2.12	0.67
2:AAA:301[B]:UDP:O2A	6:AAA:402:HOH:O	2.13	0.66
1:AAA:4:VAL:CG1	1:AAA:68:LYS:HG2	2.32	0.60
1:AAA:123:ALA:HB3	1:AAA:141:GLU:HA	1.91	0.52
1:AAA:46:ASN:OD1	1:AAA:59:LYS:HD2	2.16	0.46
1:AAA:77:SER:HB2	1:AAA:149:TYR:HB3	1.99	0.43
1:AAA:9:GLY:O	1:AAA:14:GLY:HA3	2.19	0.43
1:AAA:6:ALA:HA	1:AAA:37:VAL:O	2.19	0.42
1:AAA:65:ASN:O	1:AAA:68:LYS:HE3	2.20	0.42
1:AAA:64:LYS:HD3	1:AAA:64:LYS:HA	1.93	0.41
3:AAA:302:ACO:N7A	3:AAA:302:ACO:OAP	2.49	0.41
1:AAA:39:ILE:HA	1:AAA:55:MET:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AAA:591:HOH:O	6:AAA:628:HOH:O[3_555]	2.11	0.09

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	AAA	221/227 (97%)	211 (96%)	10 (4%)	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	AAA	180/185 (97%)	179 (99%)	1 (1%)	86 65

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	8	TYR

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

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

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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	AAA	301[B]	-	24,26,26	1.17	3 (12%)	37,40,40	1.82	8 (21%)
4	MPD	AAA	303	-	7,7,7	0.11	0	9,10,10	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ACO	AAA	302	-	45,53,53	0.93	3 (6%)	56,79,79	1.53	12 (21%)
4	MPD	AAA	304	-	7,7,7	0.15	0	9,10,10	0.40	0
2	UDP	AAA	301[A]	-	24,26,26	1.13	3 (12%)	37,40,40	2.08	9 (24%)

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	AAA	301[B]	-	-	1/16/32/32	0/2/2/2
4	MPD	AAA	303	-	-	0/5/5/5	-
3	ACO	AAA	302	-	-	3/47/67/67	0/3/3/3
4	MPD	AAA	304	-	-	1/5/5/5	-
2	UDP	AAA	301[A]	-	-	5/16/32/32	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	301[A]	UDP	C4-N3	-2.70	1.33	1.38
2	AAA	301[B]	UDP	C4-N3	-2.66	1.33	1.38
3	AAA	302	ACO	P3B-O3B	2.60	1.64	1.59
3	AAA	302	ACO	C5A-C4A	2.35	1.47	1.40
2	AAA	301[B]	UDP	C5-C4	-2.12	1.38	1.43
3	AAA	302	ACO	O4B-C1B	2.12	1.44	1.41
2	AAA	301[A]	UDP	C6-C5	2.09	1.39	1.35
2	AAA	301[B]	UDP	C6-C5	2.09	1.39	1.35
2	AAA	301[A]	UDP	C5-C4	-2.07	1.39	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	301[B]	UDP	C4-N3-C2	-5.38	119.48	126.58
2	AAA	301[A]	UDP	C4-N3-C2	-5.37	119.50	126.58
2	AAA	301[A]	UDP	O2B-PB-O3A	4.93	121.16	104.64
3	AAA	302	ACO	N3A-C2A-N1A	-4.89	121.03	128.68
2	AAA	301[B]	UDP	N3-C2-N1	4.76	121.21	114.89
2	AAA	301[A]	UDP	N3-C2-N1	4.69	121.12	114.89
2	AAA	301[A]	UDP	C5-C4-N3	4.28	121.24	114.84
2	AAA	301[B]	UDP	C5-C4-N3	4.24	121.19	114.84
3	AAA	302	ACO	CDP-CBP-CCP	3.69	114.25	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	301[A]	UDP	O3B-PB-O3A	-3.56	92.70	104.64
2	AAA	301[A]	UDP	O3B-PB-O2B	3.53	121.11	107.64
3	AAA	302	ACO	N6A-C6A-N1A	2.63	124.02	118.57
2	AAA	301[A]	UDP	O2-C2-N1	-2.55	119.39	122.79
2	AAA	301[B]	UDP	O2-C2-N1	-2.52	119.43	122.79
3	AAA	302	ACO	C5A-C6A-N6A	-2.47	116.60	120.35
3	AAA	302	ACO	O9A-P3B-O8A	2.44	116.95	107.64
2	AAA	301[A]	UDP	O4-C4-C5	-2.33	121.07	125.16
2	AAA	301[B]	UDP	O4-C4-C5	-2.32	121.07	125.16
2	AAA	301[B]	UDP	O3B-PB-O2B	2.27	116.29	107.64
3	AAA	302	ACO	C2A-N1A-C6A	2.12	122.38	118.75
3	AAA	302	ACO	O6A-CCP-CBP	-2.10	107.17	110.55
3	AAA	302	ACO	O2A-P1A-O1A	2.10	122.62	112.24
2	AAA	301[A]	UDP	C5-C6-N1	-2.07	118.35	121.81
3	AAA	302	ACO	O5A-P2A-O4A	2.06	122.44	112.24
2	AAA	301[B]	UDP	PA-O3A-PB	-2.05	125.78	132.83
3	AAA	302	ACO	O8A-P3B-O3B	-2.05	96.81	105.99
2	AAA	301[B]	UDP	C5-C6-N1	-2.05	118.38	121.81
3	AAA	302	ACO	CDP-CBP-CAP	-2.04	105.29	108.82
3	AAA	302	ACO	O8A-P3B-O7A	2.01	118.54	110.68

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	301[A]	UDP	C5'-O5'-PA-O3A
2	AAA	301[A]	UDP	O4'-C4'-C5'-O5'
4	AAA	304	MPD	O2-C2-C3-C4
2	AAA	301[A]	UDP	C3'-C4'-C5'-O5'
3	AAA	302	ACO	O4B-C4B-C5B-O5B
2	AAA	301[A]	UDP	C5'-O5'-PA-O1A
2	AAA	301[A]	UDP	C5'-O5'-PA-O2A
3	AAA	302	ACO	C3B-C4B-C5B-O5B
3	AAA	302	ACO	O9P-C9P-CAP-OAP
2	AAA	301[B]	UDP	C5'-O5'-PA-O1A

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	301[B]	UDP	2	0

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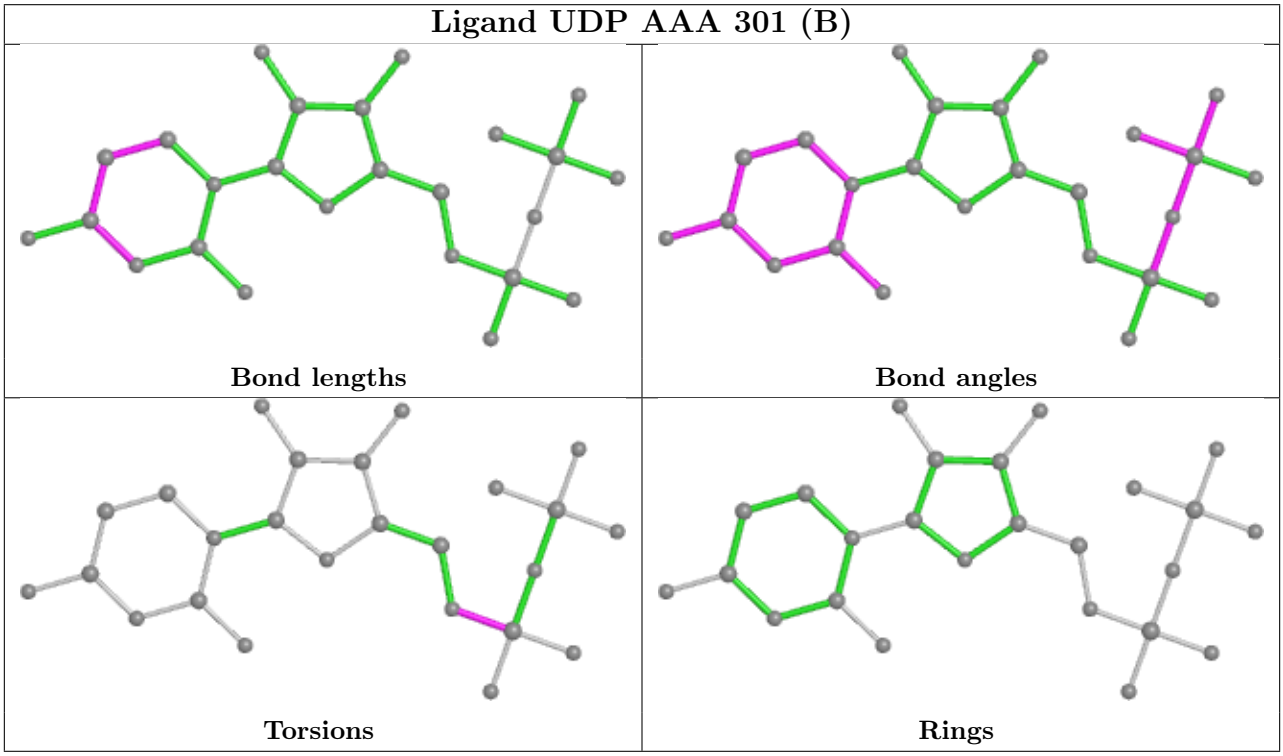
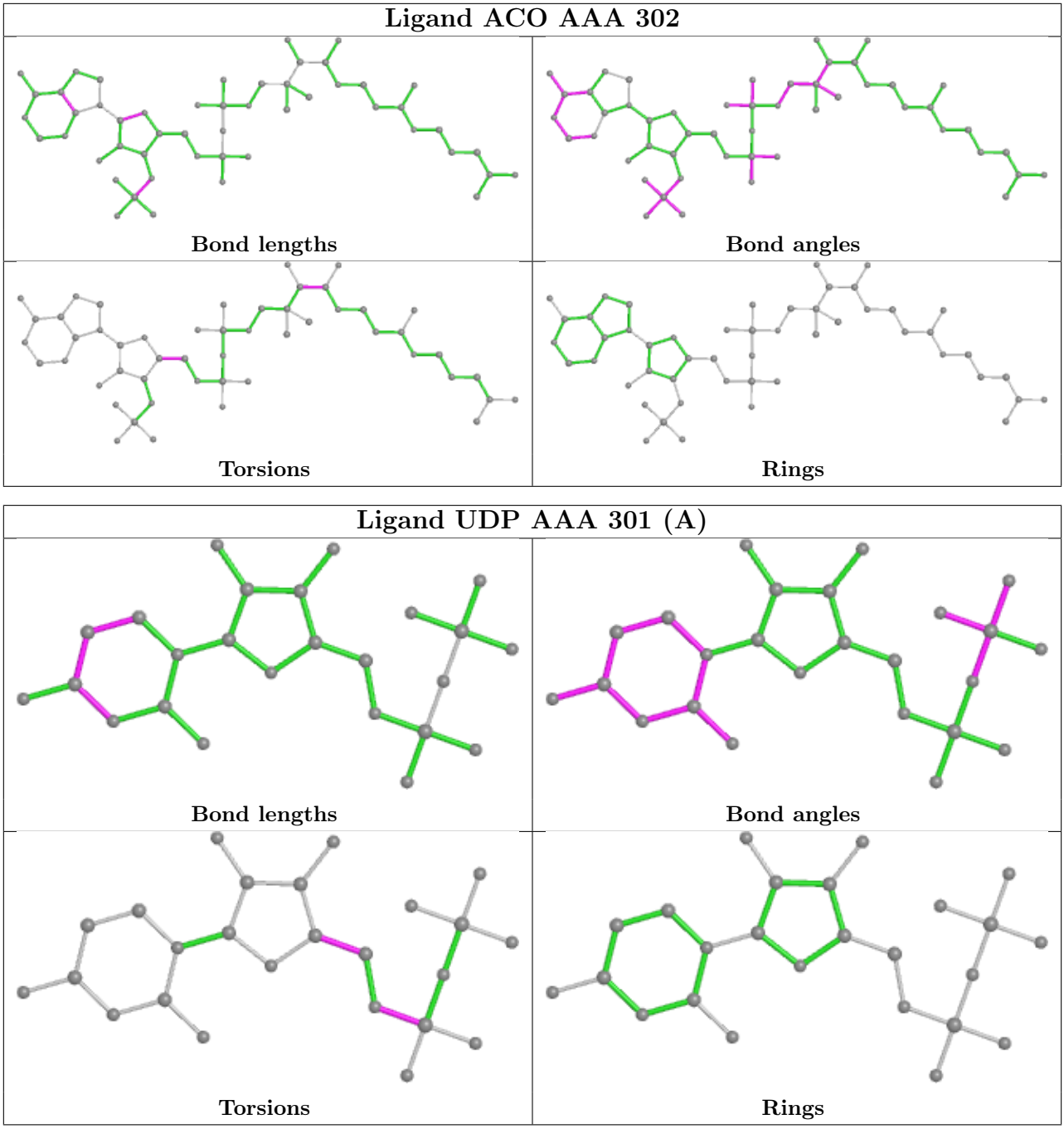
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	302	ACO	1	0

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.





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, 95^{th} 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	AAA	217/227 (95%)	-0.17	4 (1%)	68 69	4, 10, 24, 44	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	218	ASN	5.0
1	AAA	217	LEU	2.6
1	AAA	182	ASP	2.6
1	AAA	64	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, 95^{th} 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	MPD	AAA	303	8/8	0.81	0.14	27,33,36,37	0
4	MPD	AAA	304	8/8	0.86	0.24	13,15,17,19	8
2	UDP	AAA	301[A]	25/25	0.88	0.13	9,13,27,33	25

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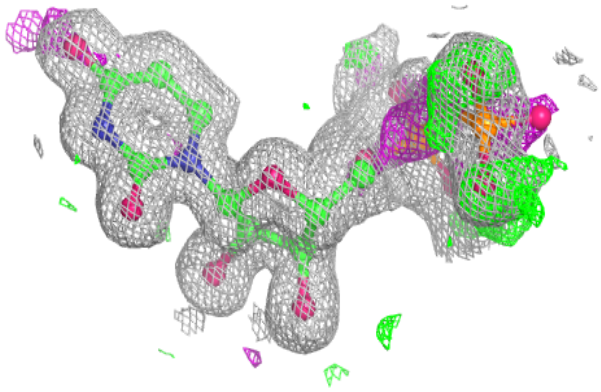
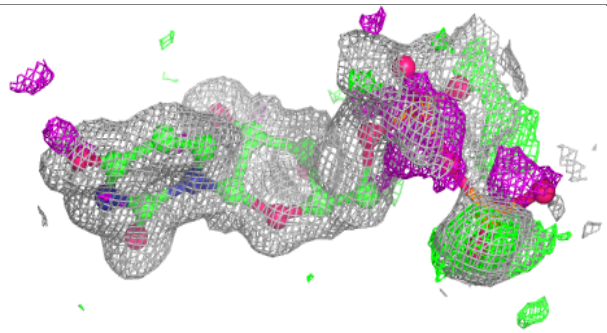
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UDP	AAA	301[B]	25/25	0.88	0.13	10,12,23,26	25
3	ACO	AAA	302	51/51	0.94	0.11	10,18,34,43	0
5	CL	AAA	305	1/1	1.00	0.07	5,5,5,5	1

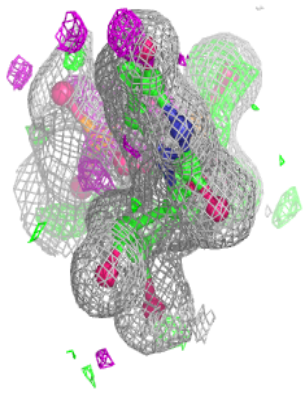
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP AAA 301 (A):

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

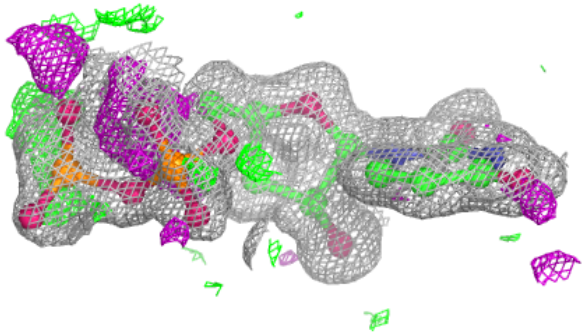






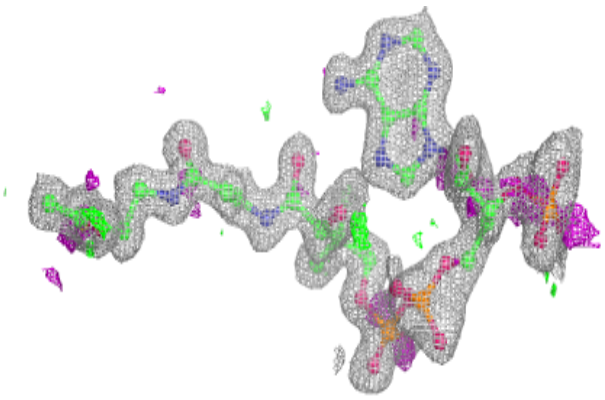
Electron density around UDP AAA 301 (B):

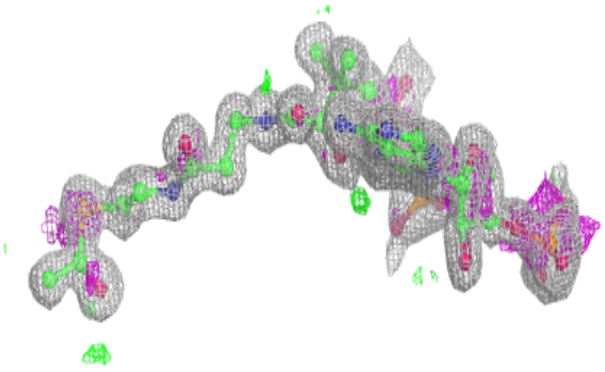
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

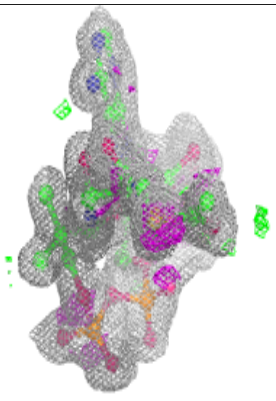


Electron density around ACO AAA 302:

$2mF_o$-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.