



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:56 PM UTC

PDB ID : 8VH8 / pdb_00008vh8
Title : Crystal structure of heparosan synthase 2 from *Pasteurella multocida* at 2.85 Å
Authors : Pedersen, L.C.; Liu, J.; Stancanelli, E.; krahn, J.M.
Deposited on : 2023-12-31
Resolution : 2.85 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

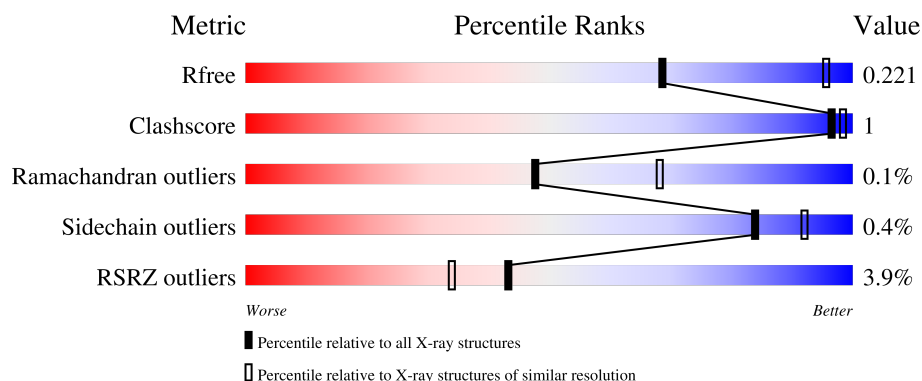
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	552	5% 90% 5% 5%
1	B	552	3% 92% . .
1	C	552	4% 92% . 6%
1	D	552	2% 93% . 5%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 32560 atoms, of which 15853 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 Heparosan synthase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	525	Total	C	H	N	O	S	0	0	0
			7850	2598	3809	673	750	20			
1	B	529	Total	C	H	N	O	S	0	0	2
			8054	2649	3927	683	774	21			
1	C	521	Total	C	H	N	O	S	0	1	0
			8010	2621	3920	683	766	20			
1	D	524	Total	C	H	N	O	S	0	1	0
			8265	2674	4085	701	783	22			

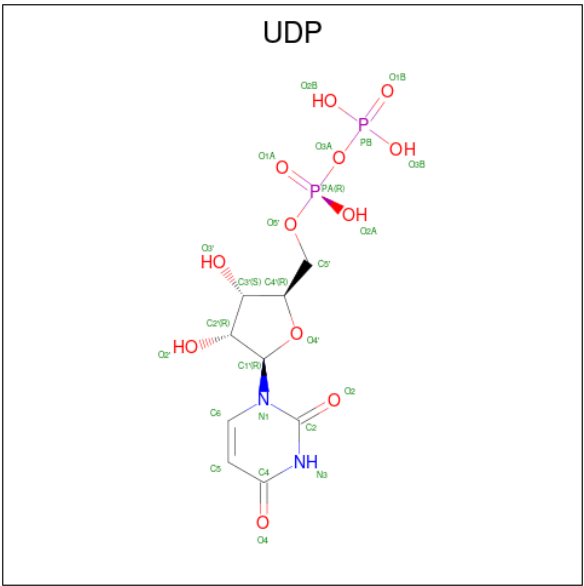
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	GLY	-	expression tag	UNP Q5SGE1
A	94	SER	-	expression tag	UNP Q5SGE1
A	95	ALA	-	expression tag	UNP Q5SGE1
A	96	ALA	-	expression tag	UNP Q5SGE1
A	97	ALA	-	expression tag	UNP Q5SGE1
B	93	GLY	-	expression tag	UNP Q5SGE1
B	94	SER	-	expression tag	UNP Q5SGE1
B	95	ALA	-	expression tag	UNP Q5SGE1
B	96	ALA	-	expression tag	UNP Q5SGE1
B	97	ALA	-	expression tag	UNP Q5SGE1
C	93	GLY	-	expression tag	UNP Q5SGE1
C	94	SER	-	expression tag	UNP Q5SGE1
C	95	ALA	-	expression tag	UNP Q5SGE1
C	96	ALA	-	expression tag	UNP Q5SGE1
C	97	ALA	-	expression tag	UNP Q5SGE1
D	93	GLY	-	expression tag	UNP Q5SGE1
D	94	SER	-	expression tag	UNP Q5SGE1
D	95	ALA	-	expression tag	UNP Q5SGE1
D	96	ALA	-	expression tag	UNP Q5SGE1
D	97	ALA	-	expression tag	UNP Q5SGE1

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	D	2	Total	Mn	0	0
			2	2		

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



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	H	N	O	P	
			36	9	11	2	12	2	
3	D	1	Total	C	H	N	O	P	
			36	9	11	2	12	2	

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na		
			1	1	0	0
4	B	1	Total	Na		
			1	1	0	0
4	C	1	Total	Na		
			1	1	0	0
4	D	1	Total	Na		
			1	1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cl		
			3	3	0	0
5	B	4	Total	Cl		
			4	4	0	0
5	C	7	Total	Cl		
			7	7	0	0
5	D	4	Total	Cl		
			4	4	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		

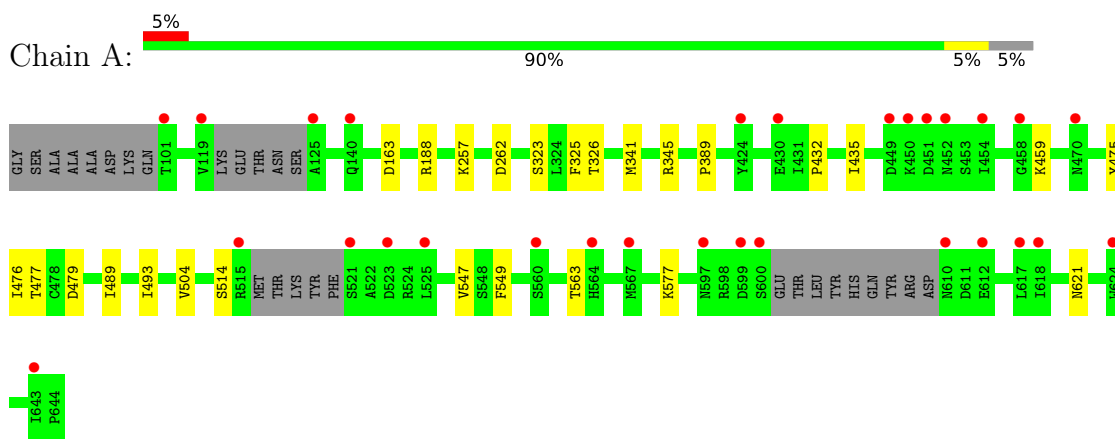
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total	O	0	0
			6	6		
8	B	5	Total	O	0	0
			5	5		
8	C	3	Total	O	0	0
			3	3		
8	D	8	Total	O	0	0
			8	8		

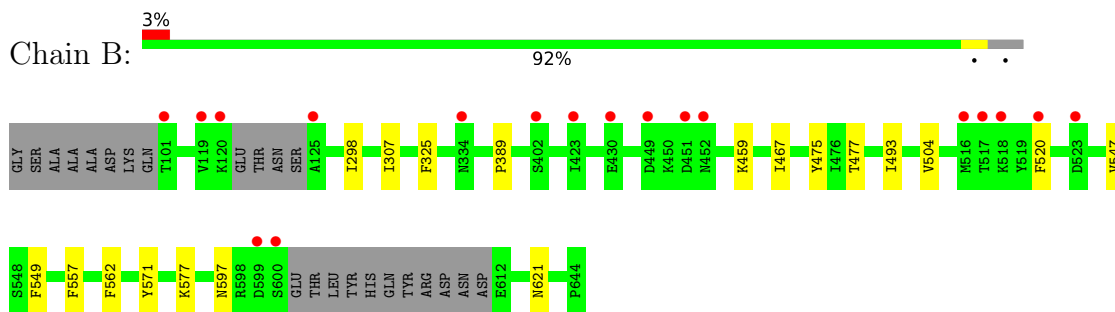
3 Residue-property plots [i](#)

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.

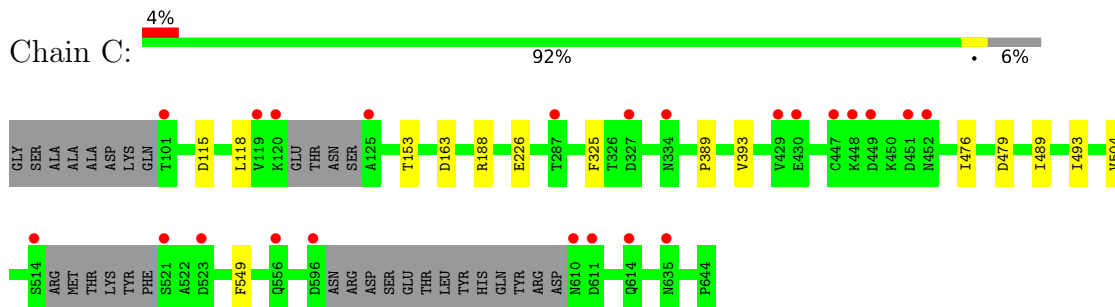
- Molecule 1: Heparosan synthase B



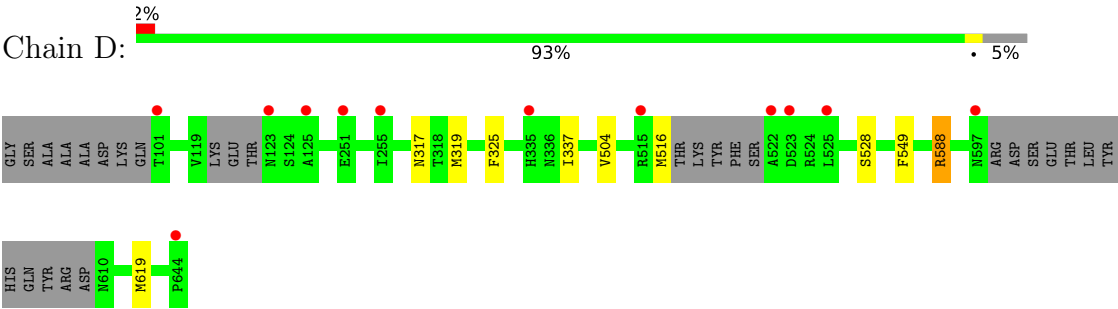
- Molecule 1: Heparosan synthase B



- Molecule 1: Heparosan synthase B



- Molecule 1: Heparosan synthase B



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	118.57Å 118.57Å 262.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.76 – 2.85 28.76 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.76-2.85) 98.7 (28.76-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.198 , 0.223 0.198 , 0.221	Depositor DCC
R_{free} test set	1986 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32560	wwPDB-VP
Average B, all atoms (Å ²)	88.0	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 33.75 % 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 7.6073e-04. 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: CL, EDO, UDP, CA, MN, NA

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	0.27	0/4128	0.45	0/5617
1	B	0.29	0/4218	0.48	0/5737
1	C	0.28	0/4178	0.45	0/5675
1	D	0.30	0/4267	0.47	0/5783
All	All	0.28	0/16791	0.46	0/22812

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4041	3809	3809	12	0
1	B	4127	3927	3925	8	0
1	C	4090	3920	3920	8	0
1	D	4180	4085	4083	5	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	50	22	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	50	22	22	0	0
3	C	50	22	22	0	0
3	D	50	22	22	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	3	0	0	0	0
5	B	4	0	0	0	0
5	C	7	0	0	0	0
5	D	4	0	0	0	0
6	B	8	12	12	0	0
6	C	4	6	6	0	0
6	D	4	6	6	0	0
7	B	1	0	0	0	0
8	A	6	0	0	1	0
8	B	5	0	0	0	0
8	C	3	0	0	1	0
8	D	8	0	0	1	0
All	All	16707	15853	15849	33	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 1.

All (33) 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:D:317:ASN:OD1	8:D:801:HOH:O	2.14	0.64
1:A:432:PRO:HD2	1:A:435:ILE:HD12	1.85	0.59
1:C:476:ILE:HD13	1:C:489:ILE:HD12	1.85	0.58
1:A:389:PRO:HG3	1:A:493:ILE:HD13	1.85	0.58
1:C:389:PRO:HG3	1:C:493:ILE:HD13	1.87	0.57
1:A:577:LYS:NZ	1:A:621:ASN:O	2.28	0.56
1:A:477:THR:OG1	1:A:547:VAL:HG22	2.07	0.54
1:C:115:ASP:HA	1:C:118:LEU:HD12	1.91	0.52
1:B:504:VAL:HG22	1:B:549:PHE:HB3	1.93	0.51
1:B:477:THR:OG1	1:B:547:VAL:HG22	2.10	0.51
1:C:153:THR:HG21	1:C:226:GLU:OE1	2.11	0.50
1:B:577:LYS:NZ	1:B:621:ASN:O	2.45	0.48
1:A:476:ILE:HD13	1:A:489:ILE:HD12	1.95	0.48
1:D:504:VAL:HG22	1:D:549:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:LYS:O	1:B:475:TYR:OH	2.33	0.47
1:C:479:ASP:OD2	8:C:801:HOH:O	2.20	0.47
1:B:298:ILE:CG2	1:B:307:ILE:HD11	2.45	0.47
1:B:467:ILE:HD12	1:B:557:PHE:HB3	1.97	0.46
1:B:562:PHE:CD1	1:B:571:TYR:HB3	2.51	0.46
1:C:393:VAL:HG13	1:C:476:ILE:HD12	1.97	0.46
1:A:323:SER:O	1:A:326:THR:HG22	2.15	0.45
1:D:528:SER:O	1:D:588:ARG:NH2	2.44	0.45
1:A:341:MET:HE2	1:A:345:ARG:HB3	1.99	0.44
1:D:516:MET:CE	1:D:619:MET:HA	2.46	0.44
1:A:459:LYS:O	1:A:475:TYR:OH	2.31	0.44
1:C:163:ASP:OD2	1:C:188:ARG:NH1	2.50	0.44
1:A:479:ASP:OD2	8:A:801:HOH:O	2.21	0.43
1:C:504:VAL:HG22	1:C:549:PHE:HB3	1.99	0.43
1:A:163:ASP:OD2	1:A:188:ARG:NH1	2.51	0.43
1:B:389:PRO:HG3	1:B:493:ILE:HD13	2.02	0.42
1:D:319:MET:HE1	1:D:337:ILE:HD13	2.01	0.42
1:A:257:LYS:NZ	1:A:262:ASP:OD1	2.52	0.41
1:A:504:VAL:HG22	1:A:549:PHE:HB3	2.03	0.41

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	517/552 (94%)	500 (97%)	16 (3%)	1 (0%)	43	62
1	B	523/552 (95%)	502 (96%)	20 (4%)	1 (0%)	43	62
1	C	514/552 (93%)	499 (97%)	15 (3%)	0	100	100
1	D	517/552 (94%)	503 (97%)	14 (3%)	0	100	100
All	All	2071/2208 (94%)	2004 (97%)	65 (3%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	520	PHE
1	A	563	THR

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	417/504 (83%)	415 (100%)	2 (0%)	81	90
1	B	439/504 (87%)	437 (100%)	2 (0%)	81	90
1	C	438/504 (87%)	437 (100%)	1 (0%)	87	95
1	D	462/504 (92%)	460 (100%)	2 (0%)	84	92
All	All	1756/2016 (87%)	1749 (100%)	7 (0%)	84	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	325	PHE
1	A	514	SER
1	B	325	PHE
1	B	597	ASN
1	C	325	PHE
1	D	325	PHE
1	D	588	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
1	A	335	HIS
1	A	356	HIS
1	A	497	ASN
1	A	621	ASN
1	B	339	GLN

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Mol	Chain	Res	Type
1	B	366	ASN
1	B	564	HIS
1	B	591	ASN
1	B	613	GLN
1	C	253	GLN
1	C	497	ASN
1	D	591	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 43 ligands modelled in this entry, 31 are monoatomic - leaving 12 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	$\# Z > 2$
6	EDO	B	712	-	3,3,3	0.41	0	2,2,2	0.28	0
3	UDP	A	702	2	25,26,26	0.62	0	38,40,40	0.81	1 (2%)
3	UDP	C	702	2	25,26,26	0.62	0	38,40,40	0.72	0
3	UDP	D	702	2	25,26,26	0.59	0	38,40,40	0.69	0
3	UDP	A	704	2	25,26,26	0.59	0	38,40,40	0.81	0
3	UDP	C	704	2	25,26,26	0.55	0	38,40,40	0.90	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UDP	D	704	2	25,26,26	0.57	0	38,40,40	0.86	0
6	EDO	B	706	-	3,3,3	0.48	0	2,2,2	0.17	0
6	EDO	D	706	-	3,3,3	0.48	0	2,2,2	0.07	0
6	EDO	C	706	-	3,3,3	0.42	0	2,2,2	0.39	0
3	UDP	B	702	2	25,26,26	0.54	0	38,40,40	0.82	0
3	UDP	B	704	2	25,26,26	0.59	0	38,40,40	0.91	1 (2%)

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
6	EDO	B	712	-	-	0/1/1/1	-
3	UDP	A	702	2	-	1/16/32/32	0/2/2/2
3	UDP	C	702	2	-	3/16/32/32	0/2/2/2
3	UDP	D	702	2	-	0/16/32/32	0/2/2/2
3	UDP	A	704	2	-	0/16/32/32	0/2/2/2
3	UDP	C	704	2	-	0/16/32/32	0/2/2/2
3	UDP	D	704	2	-	0/16/32/32	0/2/2/2
6	EDO	B	706	-	-	0/1/1/1	-
6	EDO	D	706	-	-	1/1/1/1	-
6	EDO	C	706	-	-	0/1/1/1	-
3	UDP	B	702	2	-	3/16/32/32	0/2/2/2
3	UDP	B	704	2	-	0/16/32/32	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	704	UDP	O2-C2-N1	2.15	125.60	122.80
3	C	704	UDP	O2-C2-N1	2.13	125.56	122.80
3	A	702	UDP	C3'-C2'-C1'	-2.11	97.47	101.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	UDP	C5'-O5'-PA-O1A
3	B	702	UDP	C5'-O5'-PA-O2A

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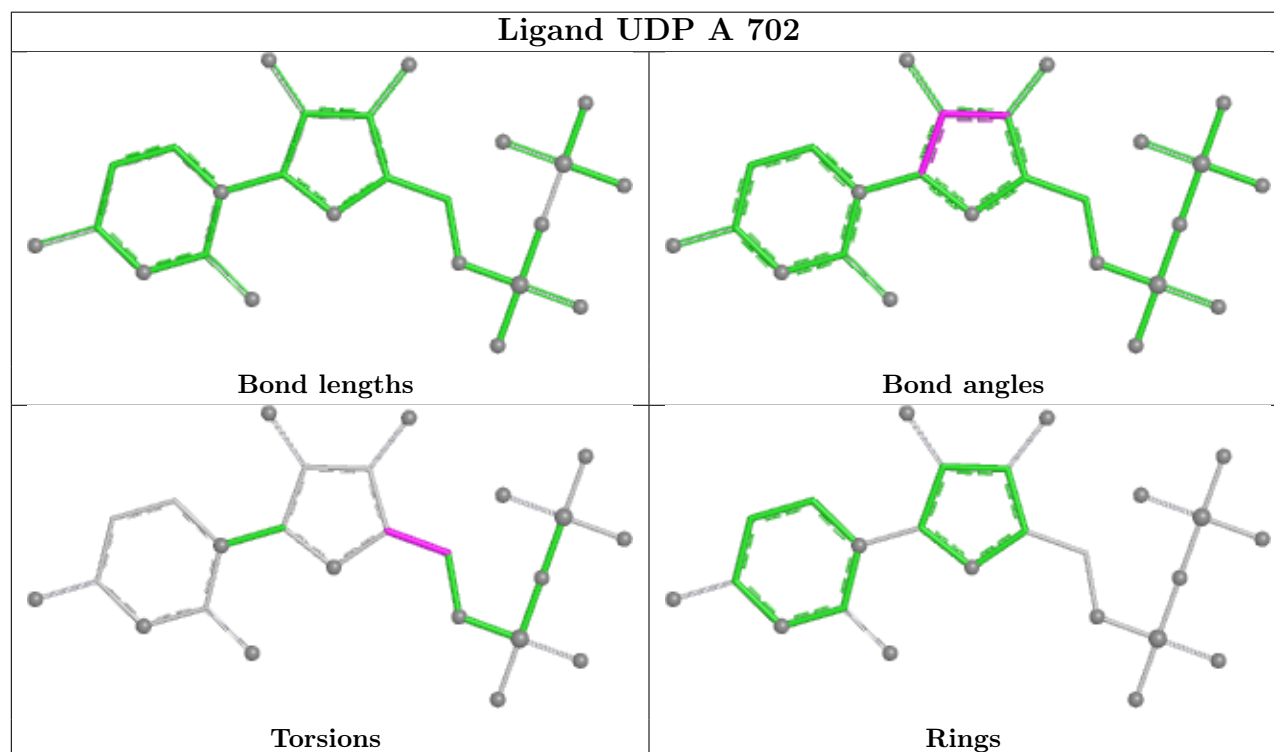
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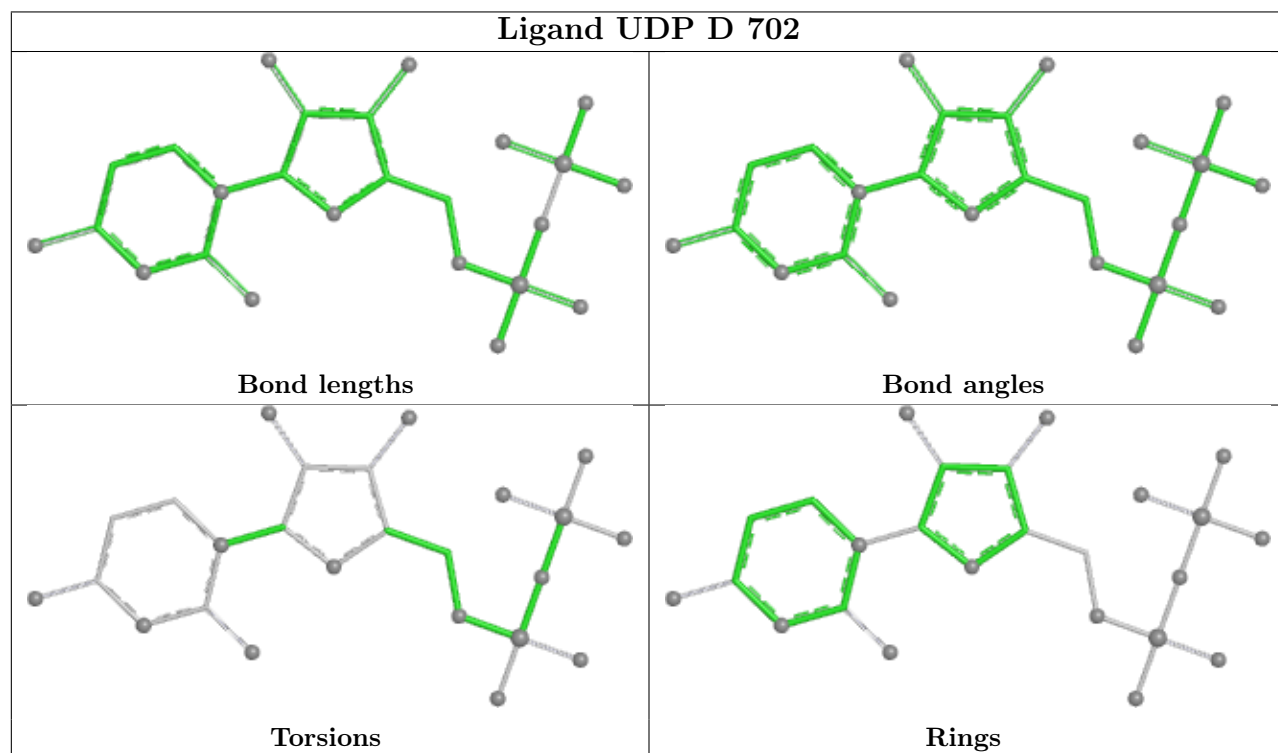
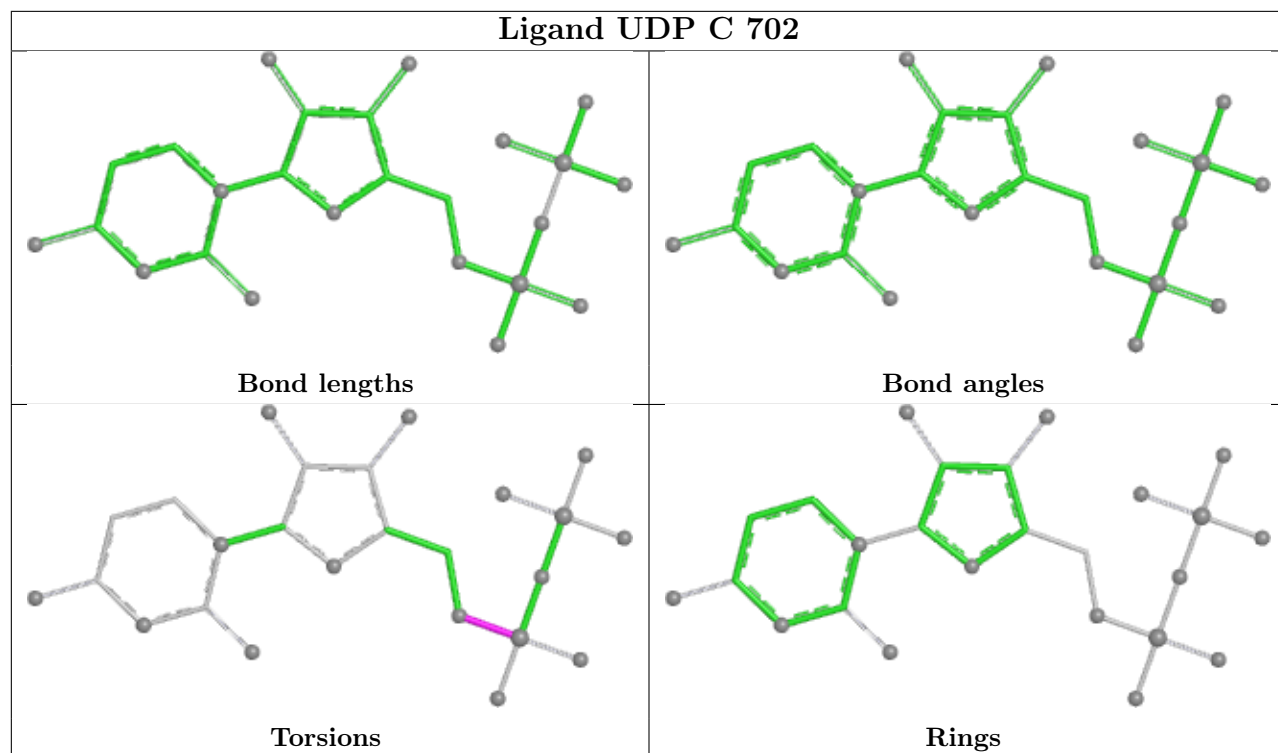
Mol	Chain	Res	Type	Atoms
3	B	702	UDP	C5'-O5'-PA-O3A
3	C	702	UDP	C5'-O5'-PA-O2A
3	C	702	UDP	C5'-O5'-PA-O1A
3	C	702	UDP	C5'-O5'-PA-O3A
6	D	706	EDO	O1-C1-C2-O2
3	A	702	UDP	O4'-C4'-C5'-O5'

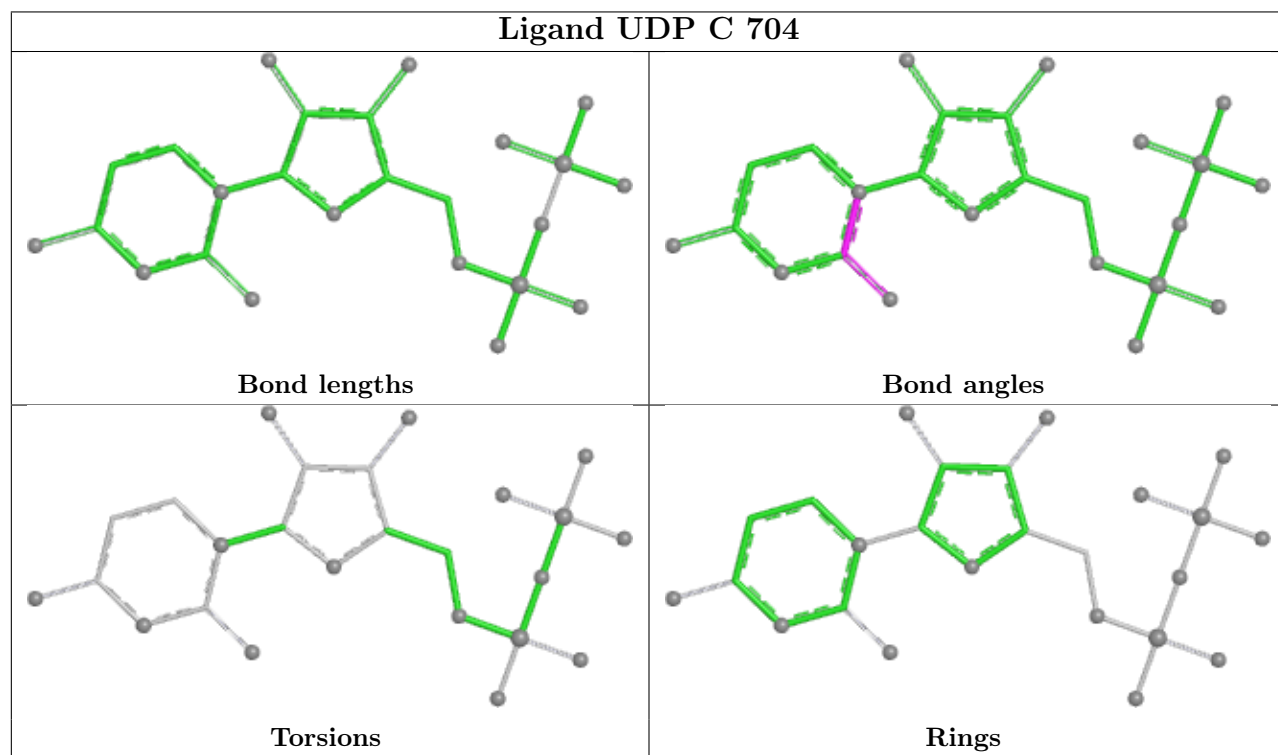
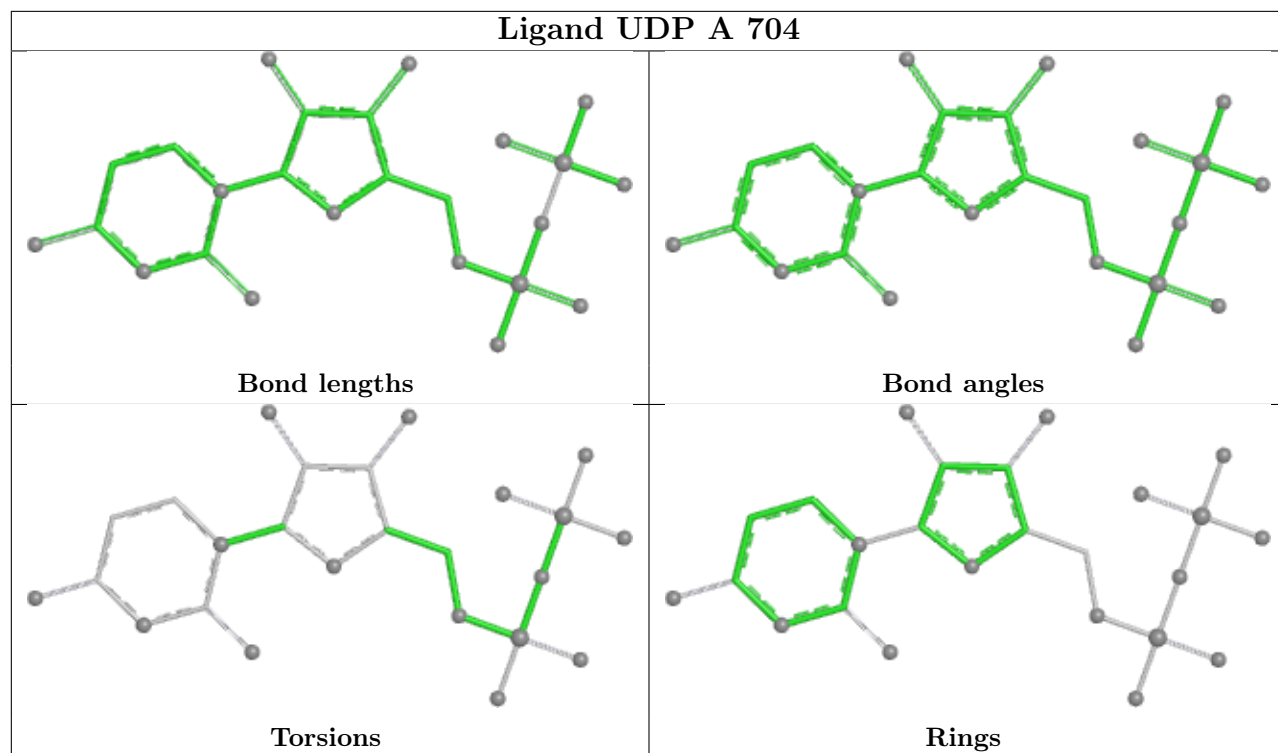
There are no ring outliers.

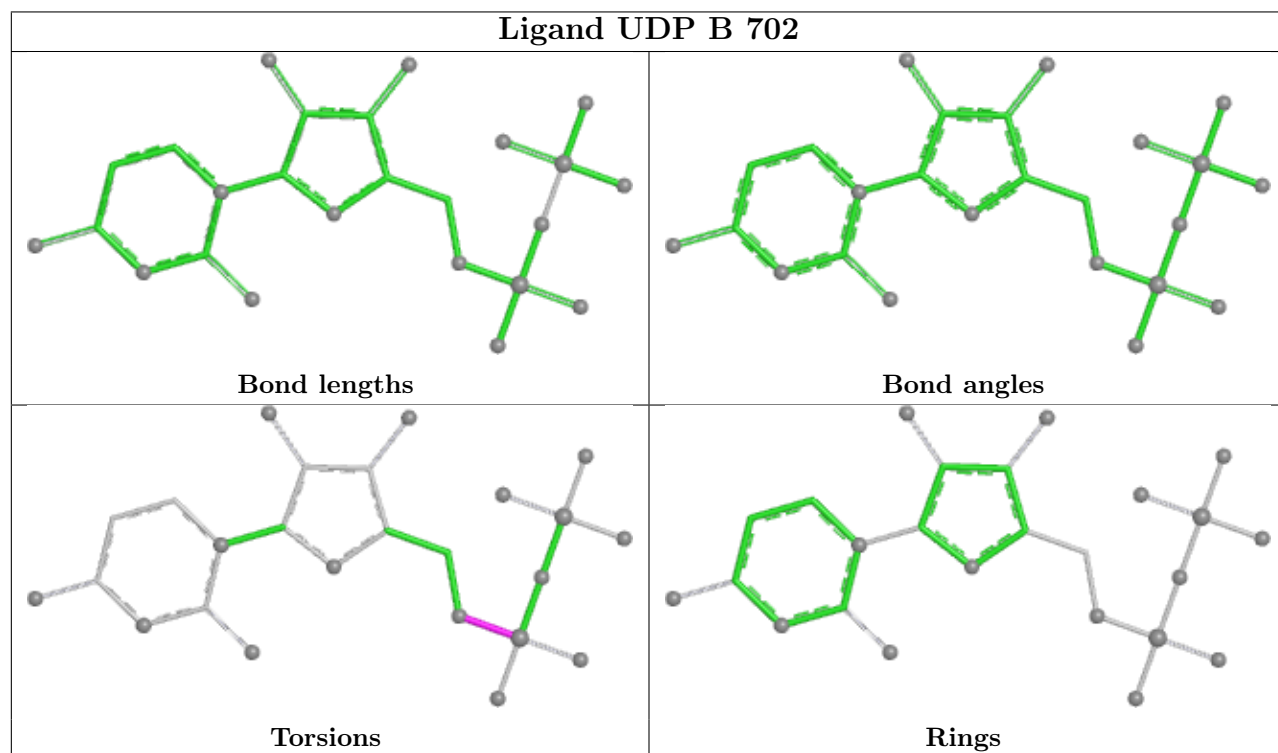
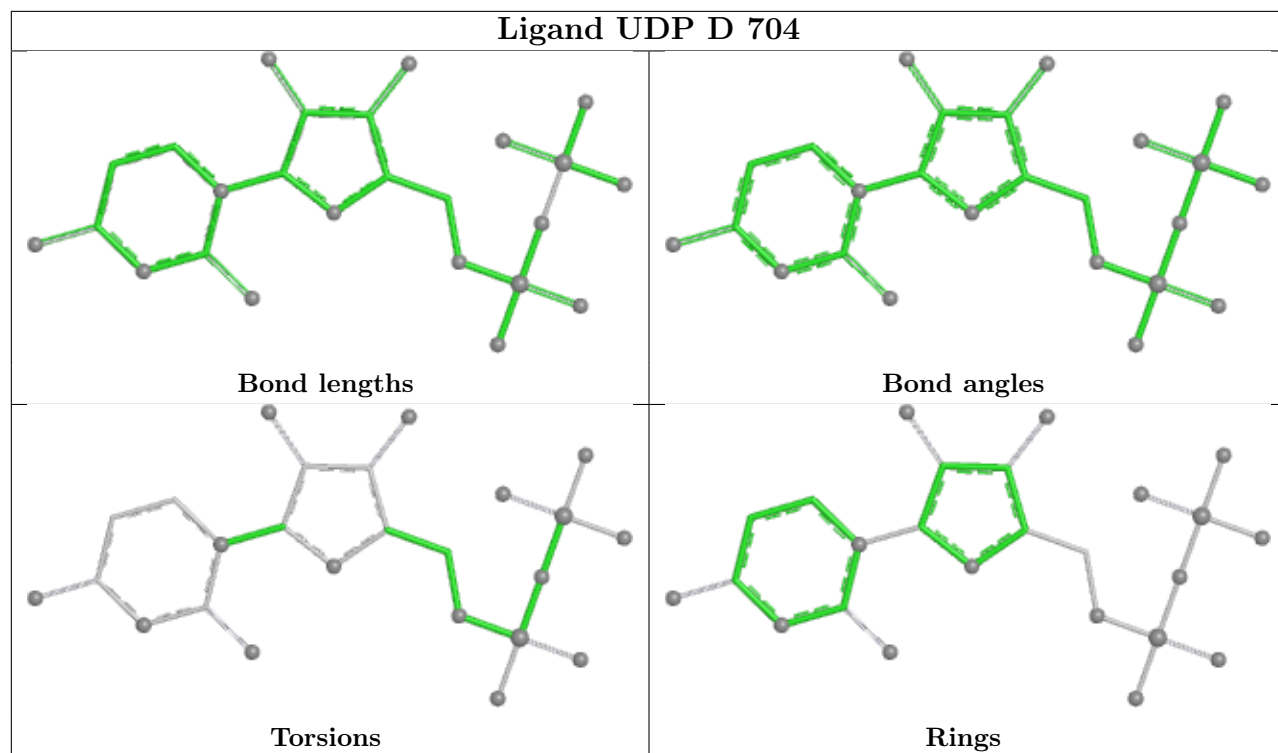
No monomer is involved in short contacts.

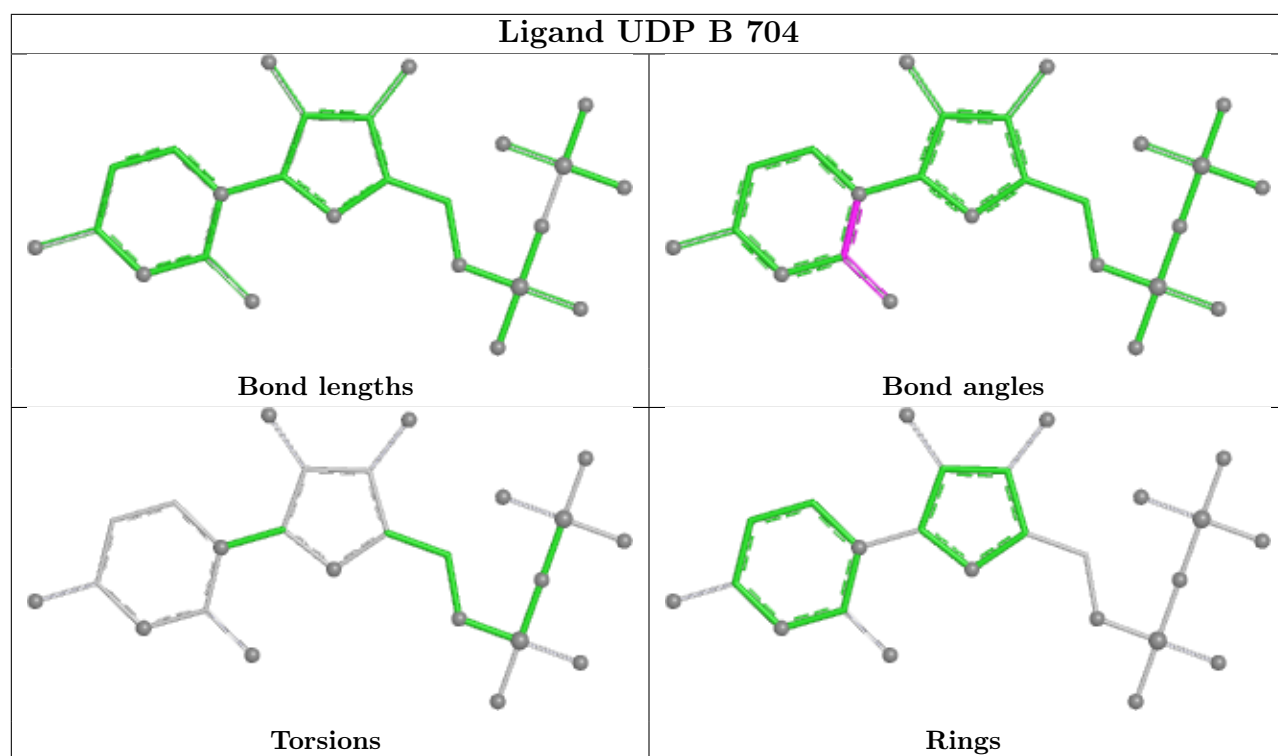
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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	525/552 (95%)	0.26	29 (5%)	30 23	61, 93, 140, 159	0
1	B	529/552 (95%)	0.09	18 (3%)	48 38	58, 82, 131, 165	0
1	C	521/552 (94%)	0.17	23 (4%)	39 30	49, 89, 134, 167	1 (0%)
1	D	524/552 (94%)	-0.11	12 (2%)	61 52	38, 76, 111, 156	1 (0%)
All	All	2099/2208 (95%)	0.10	82 (3%)	43 34	38, 85, 133, 167	2 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	SER	10.9
1	A	600	SER	8.7
1	B	101	THR	6.9
1	A	521	SER	6.6
1	C	452	ASN	6.4
1	C	101	THR	6.3
1	C	521	SER	6.1
1	A	101	THR	5.8
1	D	522	ALA	5.7
1	A	119	VAL	5.1
1	D	597	ASN	5.0
1	C	451	ASP	4.9
1	D	101	THR	4.8
1	C	523	ASP	4.7
1	A	449	ASP	4.7
1	C	447	CYS	4.6
1	B	599	ASP	4.3
1	B	120	LYS	4.1
1	B	449	ASP	4.1
1	D	123	ASN	4.1
1	C	610	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	597	ASN	4.0
1	C	635	ASN	3.9
1	A	610	ASN	3.7
1	C	596	ASP	3.5
1	A	454	ILE	3.4
1	C	449	ASP	3.4
1	A	451	ASP	3.3
1	B	125	ALA	3.3
1	B	523	ASP	3.2
1	C	430	GLU	3.2
1	B	452	ASN	3.2
1	B	516	MET	3.2
1	C	556	GLN	3.2
1	D	644	PRO	3.2
1	B	517	THR	3.1
1	A	515	ARG	3.1
1	B	451	ASP	3.1
1	A	523	ASP	3.1
1	C	125	ALA	3.1
1	D	515	ARG	3.0
1	A	567	MET	3.0
1	B	430	GLU	2.9
1	A	452	ASN	2.9
1	A	470	ASN	2.9
1	A	430	GLU	2.8
1	A	525	LEU	2.8
1	C	334	ASN	2.8
1	D	523	ASP	2.8
1	C	429	VAL	2.8
1	D	251	GLU	2.7
1	B	520	PHE	2.7
1	C	327	ASP	2.7
1	D	125	ALA	2.7
1	B	402	SER	2.7
1	C	514	SER	2.7
1	A	599	ASP	2.7
1	B	423	ILE	2.6
1	A	125	ALA	2.5
1	C	119	VAL	2.5
1	B	334	ASN	2.4
1	A	450	LYS	2.4
1	C	614	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	448	LYS	2.3
1	A	424	TYR	2.3
1	A	140	GLN	2.3
1	A	560	SER	2.3
1	A	643	ILE	2.3
1	D	335	HIS	2.3
1	A	617	LEU	2.2
1	C	287	THR	2.2
1	D	255	ILE	2.2
1	A	564	HIS	2.2
1	B	119	VAL	2.2
1	C	120	LYS	2.2
1	A	624	TRP	2.2
1	A	618	ILE	2.2
1	A	458	GLY	2.1
1	D	525	LEU	2.1
1	A	612	GLU	2.1
1	C	611	ASP	2.0
1	B	518	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CL	B	707	1/1	0.85	0.11	110,110,110,110	0
5	CL	D	707	1/1	0.86	0.14	98,98,98,98	0
4	NA	A	705	1/1	0.87	0.16	67,67,67,67	0
6	EDO	B	706	4/4	0.89	0.17	58,70,75,77	0

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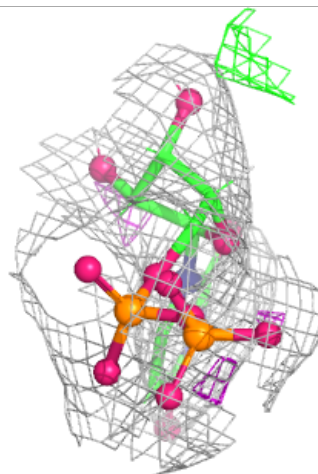
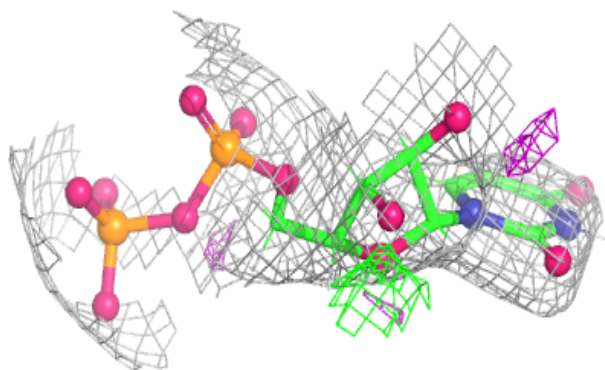
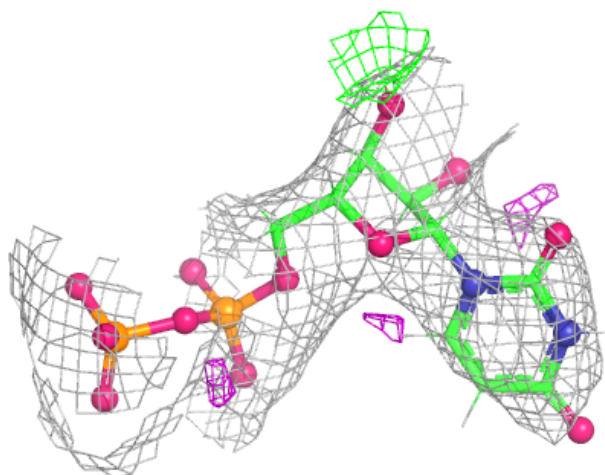
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	D	706	4/4	0.89	0.12	58,69,74,74	0
3	UDP	A	702	25/25	0.90	0.11	109,119,143,149	0
5	CL	A	708	1/1	0.90	0.10	87,87,87,87	0
7	CA	B	708	1/1	0.90	0.10	85,85,85,85	0
3	UDP	C	702	25/25	0.91	0.10	102,112,135,145	0
3	UDP	B	702	25/25	0.91	0.10	91,96,116,119	0
4	NA	B	705	1/1	0.91	0.18	64,64,64,64	0
4	NA	C	705	1/1	0.92	0.07	72,72,72,72	0
5	CL	B	711	1/1	0.92	0.08	83,83,83,83	0
6	EDO	B	712	4/4	0.93	0.10	56,67,70,74	0
6	EDO	C	706	4/4	0.93	0.17	64,77,78,79	0
5	CL	D	709	1/1	0.95	0.09	65,65,65,65	0
5	CL	C	709	1/1	0.95	0.08	74,74,74,74	0
5	CL	C	710	1/1	0.95	0.10	73,73,73,73	0
5	CL	C	712	1/1	0.95	0.08	81,81,81,81	0
5	CL	C	713	1/1	0.95	0.06	73,73,73,73	0
5	CL	C	707	1/1	0.95	0.10	71,71,71,71	0
3	UDP	A	704	25/25	0.96	0.08	59,70,78,81	0
5	CL	A	706	1/1	0.96	0.07	71,71,71,71	0
5	CL	C	711	1/1	0.96	0.06	87,87,87,87	0
3	UDP	D	702	25/25	0.96	0.07	75,83,100,105	0
2	MN	A	701	1/1	0.97	0.04	110,110,110,110	0
5	CL	B	709	1/1	0.97	0.11	66,66,66,66	0
5	CL	B	710	1/1	0.97	0.07	68,68,68,68	0
5	CL	D	708	1/1	0.97	0.06	61,61,61,61	0
2	MN	B	701	1/1	0.97	0.05	97,97,97,97	0
2	MN	C	701	1/1	0.97	0.04	105,105,105,105	0
5	CL	C	708	1/1	0.97	0.06	69,69,69,69	0
3	UDP	B	704	25/25	0.97	0.07	53,65,71,73	0
2	MN	C	703	1/1	0.97	0.05	74,74,74,74	0
3	UDP	C	704	25/25	0.97	0.07	60,68,77,79	0
5	CL	A	707	1/1	0.98	0.07	72,72,72,72	0
2	MN	D	703	1/1	0.98	0.04	66,66,66,66	0
4	NA	D	705	1/1	0.98	0.04	62,62,62,62	0
3	UDP	D	704	25/25	0.98	0.06	50,58,66,69	0
5	CL	D	710	1/1	0.98	0.07	62,62,62,62	0
2	MN	A	703	1/1	0.99	0.03	72,72,72,72	0
2	MN	B	703	1/1	0.99	0.04	68,68,68,68	0
2	MN	D	701	1/1	0.99	0.03	81,81,81,81	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.

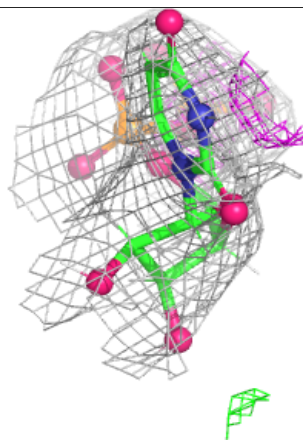
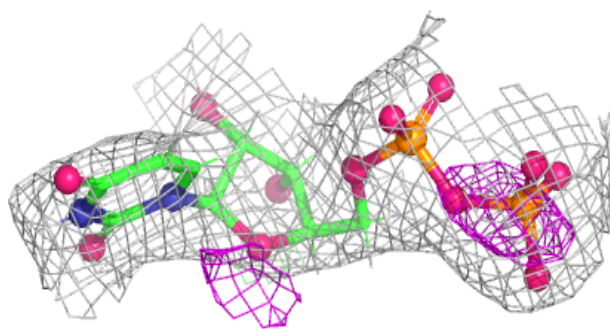
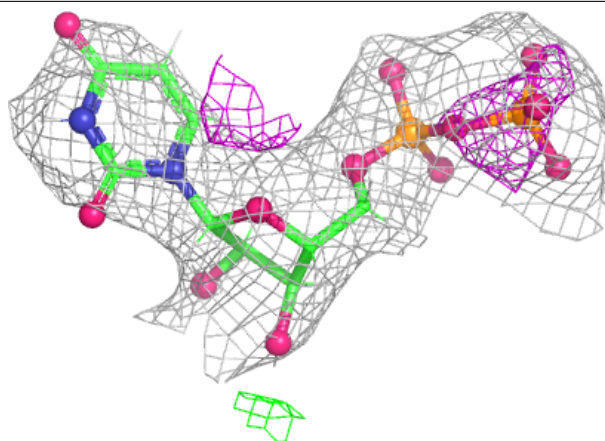
Electron density around UDP A 702:

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



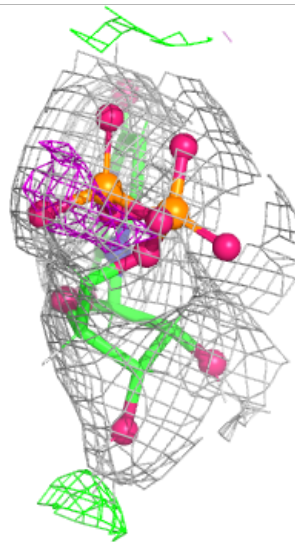
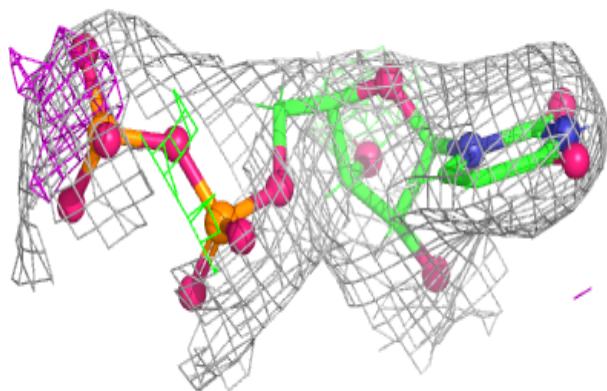
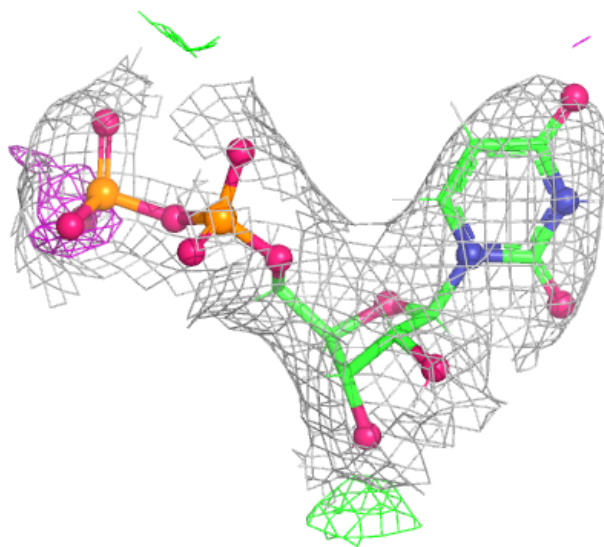
Electron density around UDP C 702:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



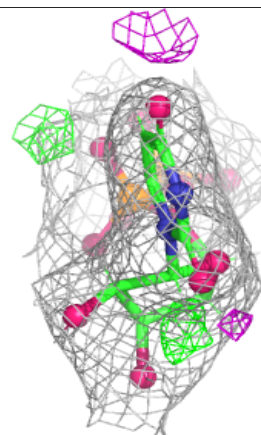
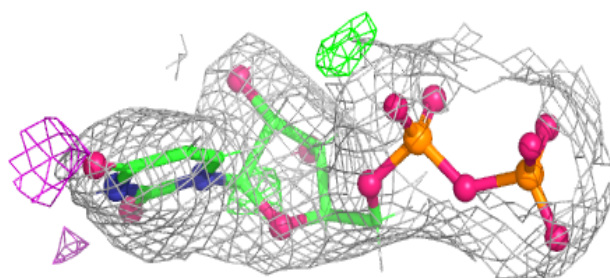
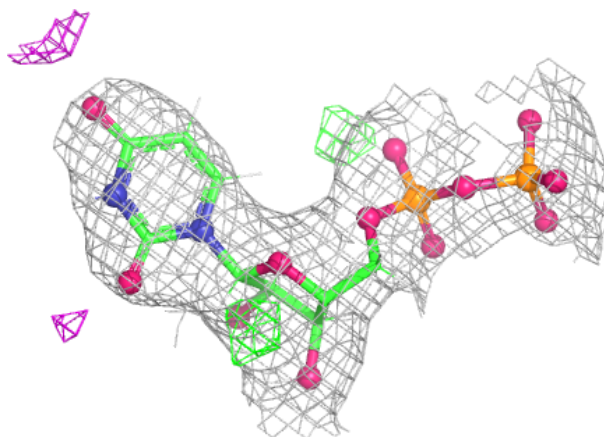
Electron density around UDP B 702:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



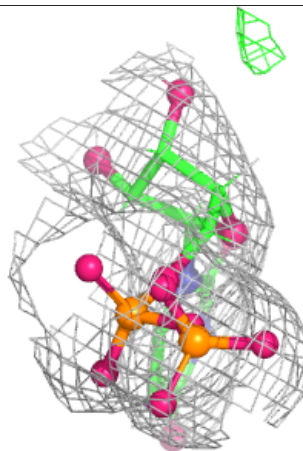
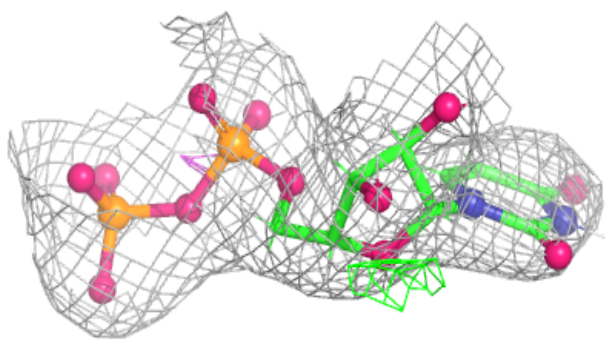
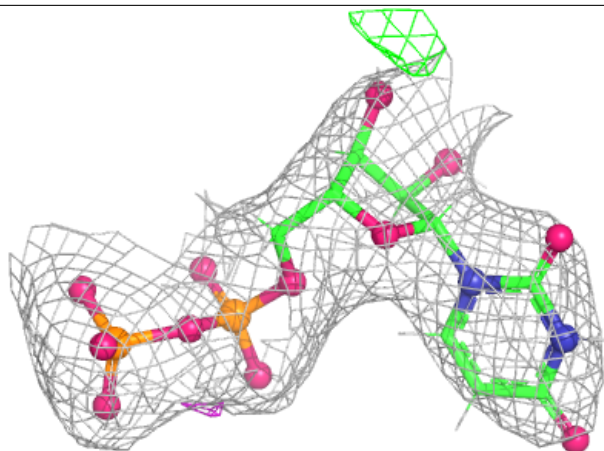
Electron density around UDP A 704:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



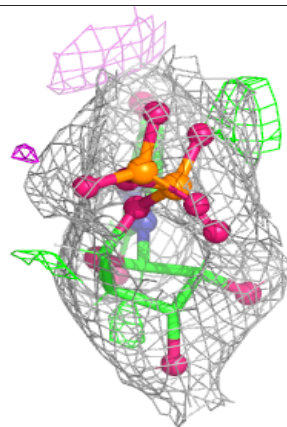
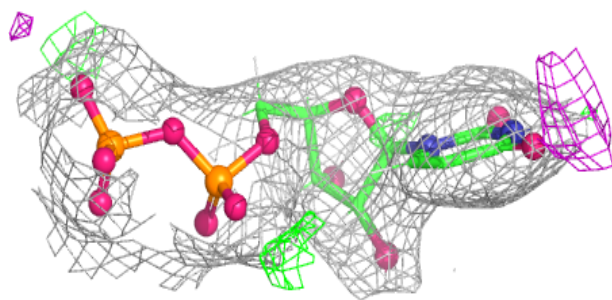
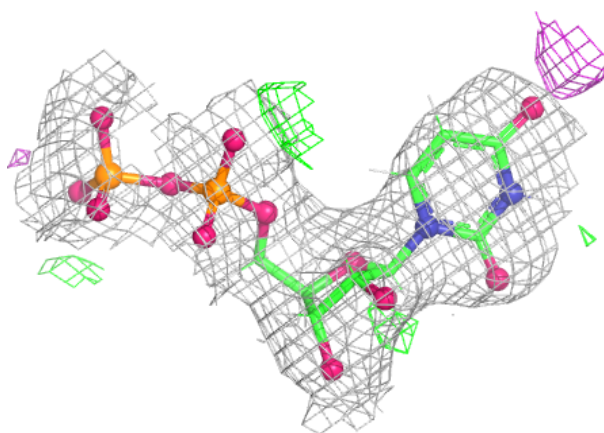
Electron density around UDP D 702:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



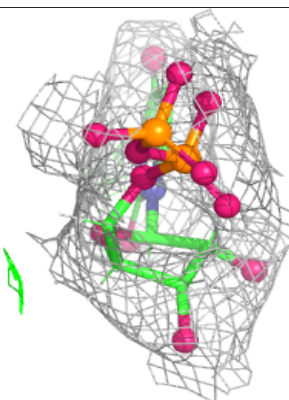
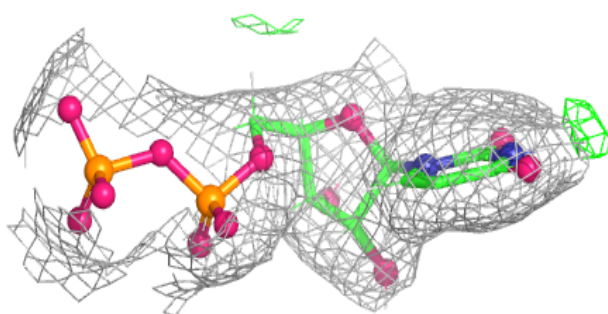
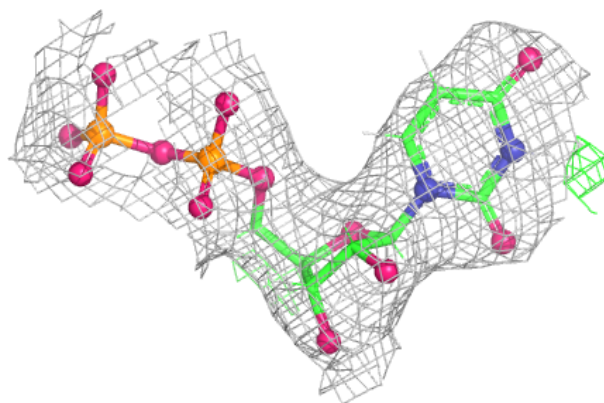
Electron density around UDP B 704:

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

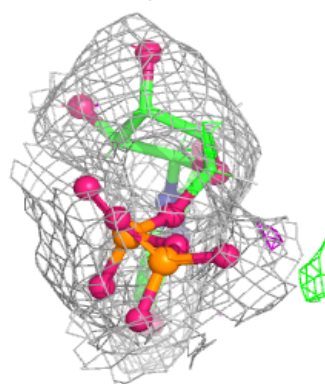
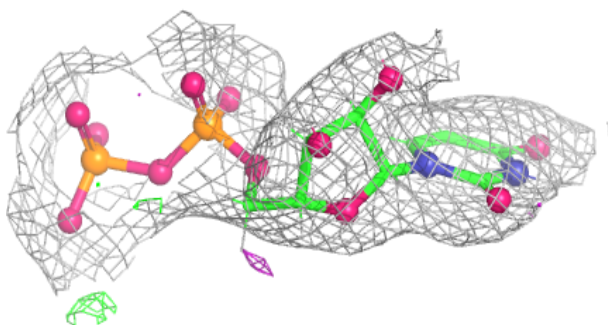
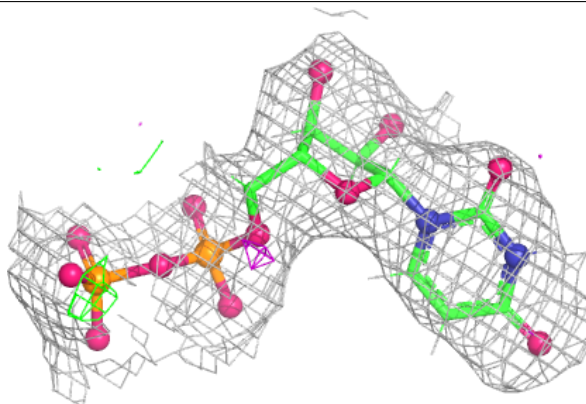


Electron density around UDP C 704:

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

**Electron density around UDP D 704:**

$2mF_o-DF_c$ (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.