



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 07:48 pm BST

PDB ID : 2WTX  
Title : Insight into the mechanism of enzymatic glycosyltransfer with retention through the synthesis and analysis of bisubstrate glycomimetics of trehalos e-6-phosphate synthase  
Authors : Errey, J.C.; Lee, S.S.; Gibson, R.P.; Martinez-Fleites, C.; Barry, C.S.; Jung, P.M.J.; OSullivan, A.; Davis, B.G.; Davies, G.J.  
Deposited on : 2009-09-25  
Resolution : 2.20 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](mailto: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.

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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	:	2.11
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)	:	2.11

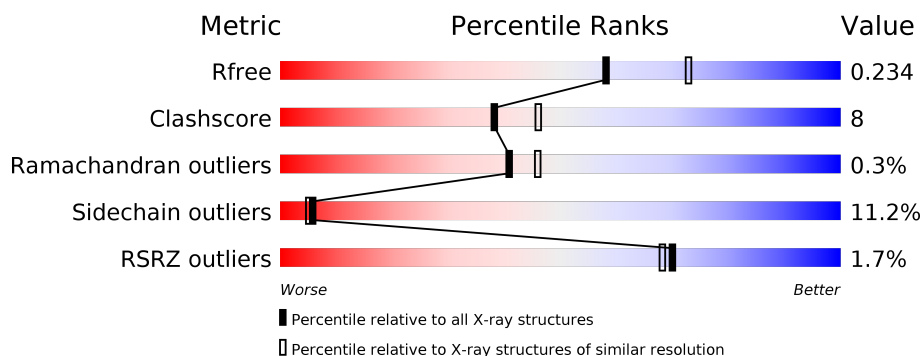
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	474	<div> <div style="width: 77%;"></div> <div style="width: 15%;"></div> <div style="width: 8%;"></div> <div style="width: 0%;"></div> </div>
1	B	474	<div> <div style="width: 78%;"></div> <div style="width: 16%;"></div> <div style="width: 6%;"></div> <div style="width: 0%;"></div> </div>
1	C	474	<div> <div style="width: 70%;"></div> <div style="width: 19%;"></div> <div style="width: 7%;"></div> <div style="width: 4%;"></div> </div>
1	D	474	<div> <div style="width: 79%;"></div> <div style="width: 13%;"></div> <div style="width: 6%;"></div> <div style="width: 2%;"></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	1458	-	-	X	X
2	EDO	A	1459	-	-	X	-
2	EDO	B	1459	-	-	X	-

## 2 Entry composition [i](#)

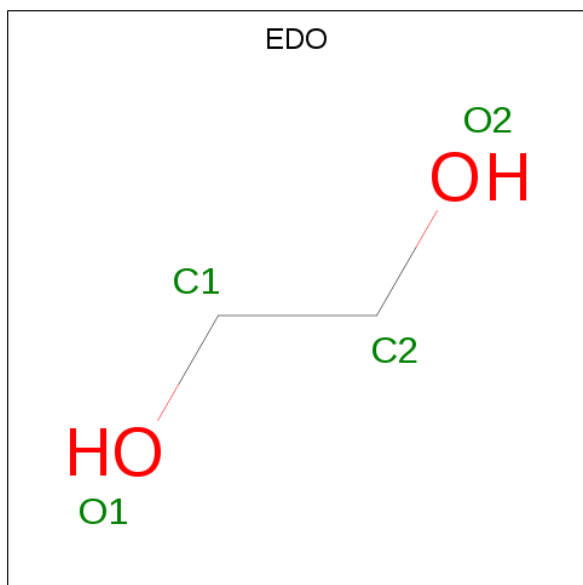
There are 5 unique types of molecules in this entry. The entry contains 15336 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALPHA, ALPHA-TREHALOSE-PHOSPHATE SYNTHASE [UDP-FORMING].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	3	0
			3674	2359	643	665	7			
1	B	454	Total	C	N	O	S	0	1	0
			3644	2343	633	661	7			
1	C	440	Total	C	N	O	S	0	1	0
			3545	2279	619	640	7			
1	D	457	Total	C	N	O	S	0	0	0
			3660	2349	638	666	7			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



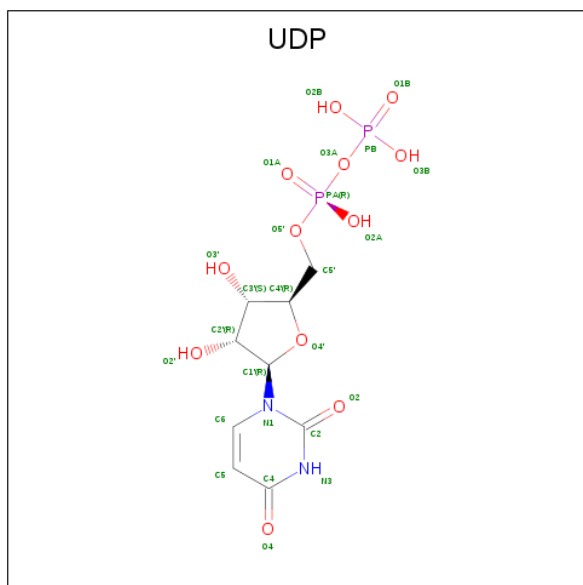
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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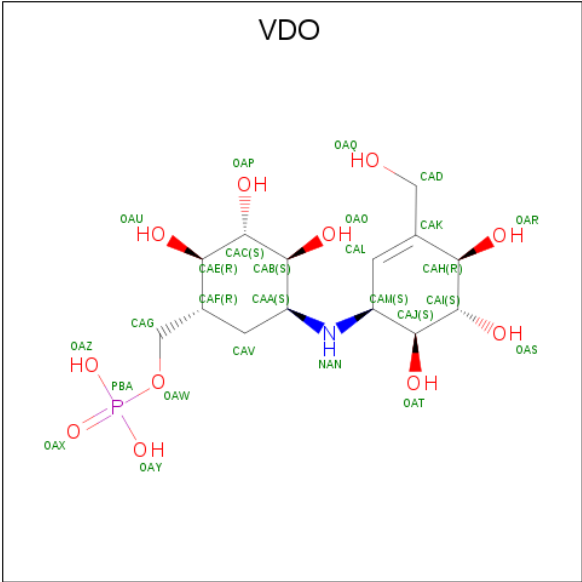
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).



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

- Molecule 4 is [(1R,2R,3S,4S,5S)-2,3,4-TRIHYDROXY-5-{[(1S,4R,5S,6S)-4,5,6-TRIHYDROXY-3-(HYDROXYMETHYL)CYCLOHEX-2-EN-1-YL]AMINO}CYCLOHEXYL]METHYL DIHYDROGEN PHOSPHATE (three-letter code: VDO) (formula:  $C_{14}H_{26}NO_{11}P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	14	1	11	1		
4	B	1	Total	C	N	O	P	0	0
			27	14	1	11	1		
4	C	1	Total	C	N	O	P	0	0
			27	14	1	11	1		
4	D	1	Total	C	N	O	P	0	0
			27	14	1	11	1		

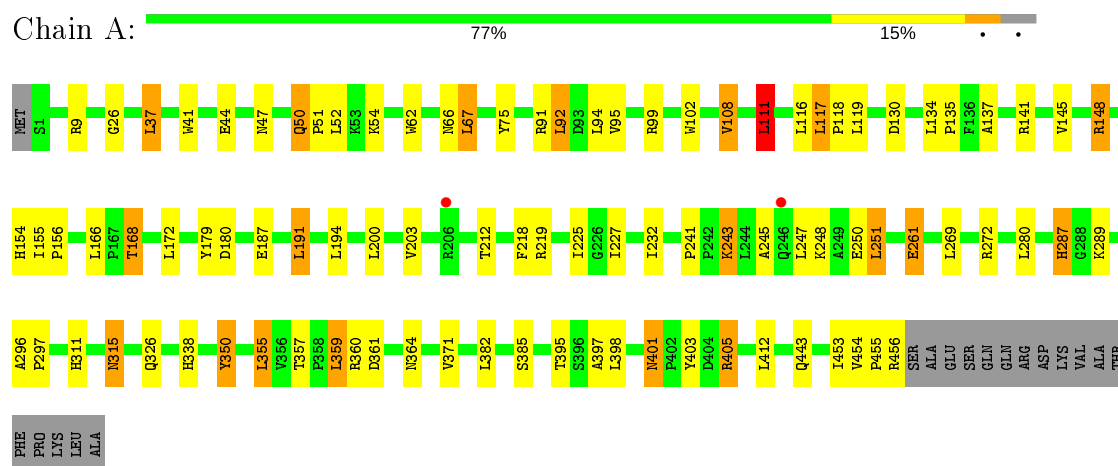
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	202	Total	O	0	0
			202	202		
5	B	152	Total	O	0	0
			152	152		
5	C	76	Total	O	0	0
			76	76		
5	D	155	Total	O	0	0
			155	155		

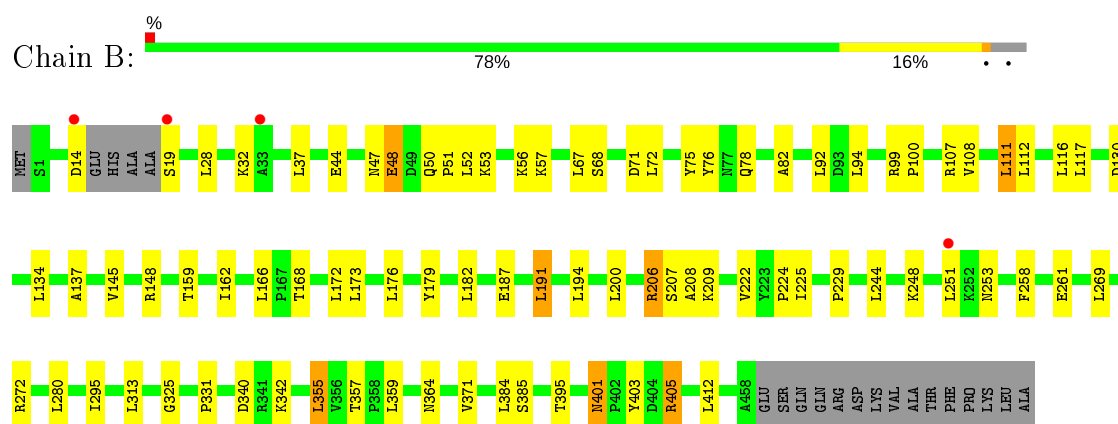
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

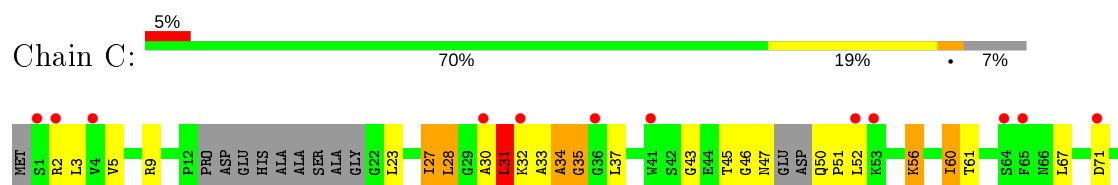
- Molecule 1: ALPHA, ALPHA-TREHALOSE-PHOSPHATE SYNTHASE [UDP-FORMING]

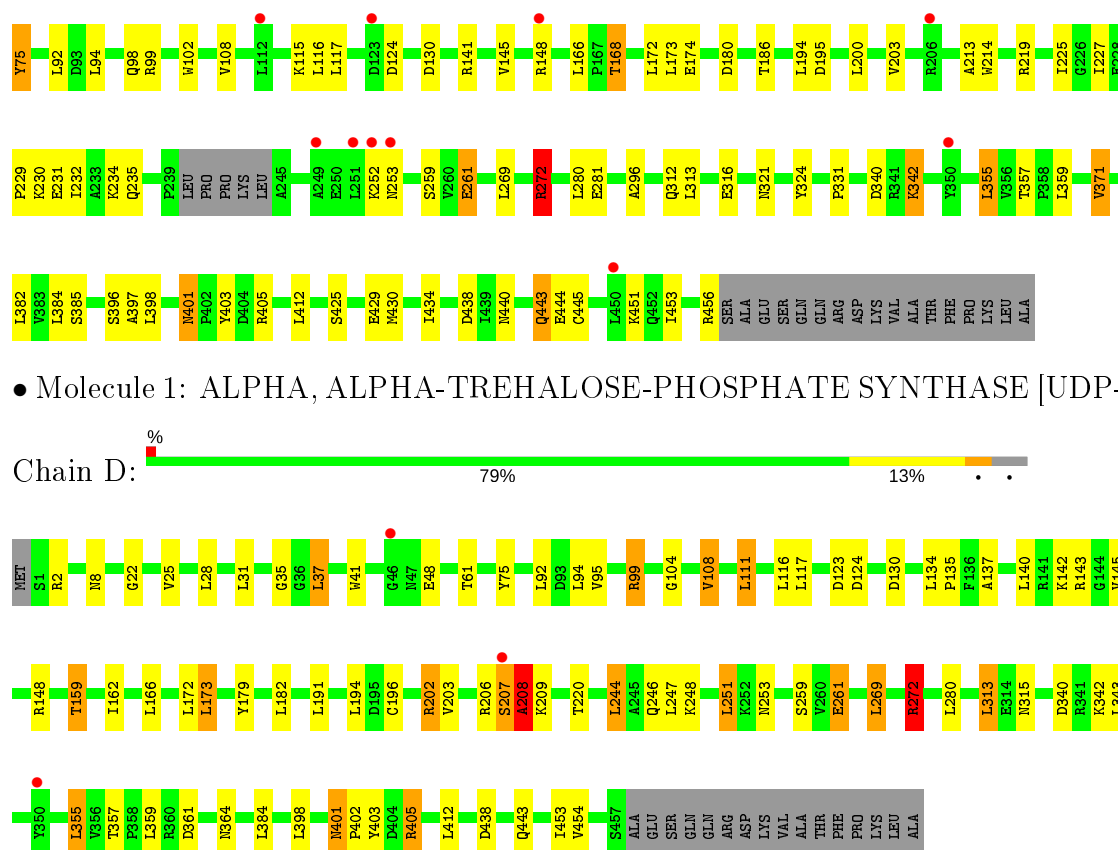


- Molecule 1: ALPHA, ALPHA-TREHALOSE-PHOSPHATE SYNTHASE [UDP-FORMING]

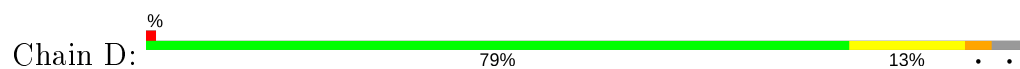


- Molecule 1: ALPHA, ALPHA-TREHALOSE-PHOSPHATE SYNTHASE [UDP-FORMING]





- Molecule 1: ALPHA, ALPHA-TREHALOSE-PHOSPHATE SYNTHASE [UDP-FORMING]





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.52Å 120.29Å 173.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.91 – 2.20 98.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (98.91-2.20) 99.9 (98.91-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.70 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.195 , 0.235 0.196 , 0.234	Depositor DCC
$R_{free}$ test set	5583 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15336	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, EDO, VDO

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	0.60	0/3777	0.72	3/5135 (0.1%)
1	B	0.62	5/3739 (0.1%)	0.76	5/5082 (0.1%)
1	C	0.60	6/3634 (0.2%)	0.67	4/4934 (0.1%)
1	D	0.65	3/3753 (0.1%)	0.77	10/5103 (0.2%)
All	All	0.62	14/14903 (0.1%)	0.73	22/20254 (0.1%)

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	B	0	1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	208	ALA	N-CA	-8.89	1.28	1.46
1	C	34	ALA	CA-CB	-7.18	1.37	1.52
1	D	206	ARG	CZ-NH2	-6.93	1.24	1.33
1	B	209	LYS	CE-NZ	-6.56	1.32	1.49
1	C	33	ALA	CA-CB	-6.55	1.38	1.52

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	ARG	NE-CZ-NH1	13.53	127.06	120.30
1	B	206	ARG	NE-CZ-NH2	-13.00	113.80	120.30
1	C	31	LEU	CB-CG-CD2	-10.10	93.83	111.00
1	D	207	SER	CB-CA-C	9.69	128.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	LEU	CA-CB-CG	8.82	135.59	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	208	ALA	Peptide

## 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	3674	0	3650	58	0
1	B	3644	0	3619	34	0
1	C	3545	0	3523	65	0
1	D	3660	0	3629	61	0
2	A	12	0	18	9	0
2	B	8	0	12	4	0
3	A	25	0	11	0	0
3	B	25	0	11	1	0
3	C	25	0	11	0	0
3	D	25	0	11	0	0
4	A	27	0	24	3	0
4	B	27	0	24	3	0
4	C	27	0	24	2	0
4	D	27	0	24	1	0
5	A	202	0	0	8	0
5	B	152	0	0	2	0
5	C	76	0	0	4	0
5	D	155	0	0	0	0
All	All	15336	0	14591	222	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 8.

The worst 5 of 222 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:207:SER:CB	1:D:208:ALA:HB3	1.67	1.21
1:D:207:SER:HB2	1:D:208:ALA:HB3	1.27	1.15
1:D:207:SER:CB	1:D:208:ALA:CB	2.29	1.10
1:D:92:LEU:HD11	1:D:162:ILE:HG23	1.32	1.10
1:C:31:LEU:CD1	1:C:31:LEU:C	2.28	1.00

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	457/474 (96%)	441 (96%)	15 (3%)	1 (0%)	47	55
1	B	451/474 (95%)	429 (95%)	21 (5%)	1 (0%)	47	55
1	C	433/474 (91%)	417 (96%)	16 (4%)	0	100	100
1	D	455/474 (96%)	437 (96%)	15 (3%)	3 (1%)	22	22
All	All	1796/1896 (95%)	1724 (96%)	67 (4%)	5 (0%)	41	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	208	ALA
1	B	364	ASN
1	A	364	ASN
1	D	364	ASN
1	D	438	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	387/399 (97%)	342 (88%)	45 (12%)	5	5
1	B	384/399 (96%)	342 (89%)	42 (11%)	6	5
1	C	373/399 (94%)	326 (87%)	47 (13%)	4	3
1	D	385/399 (96%)	347 (90%)	38 (10%)	8	7
All	All	1529/1596 (96%)	1357 (89%)	172 (11%)	6	5

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	261	GLU
1	C	75	TYR
1	D	261	GLU
1	B	355	LEU
1	C	27	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	78	GLN
1	B	401	ASN
1	D	256	ASN
1	B	175	GLN
1	A	175	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

13 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	EDO	B	1460	-	3,3,3	0.54	0	2,2,2	0.40	0
4	VDO	D	1459	-	28,28,28	1.62	5 (17%)	31,42,42	1.15	4 (12%)
3	UDP	C	1457	-	20,26,26	1.13	1 (5%)	25,40,40	0.96	2 (8%)
3	UDP	A	1460	-	20,26,26	1.06	1 (5%)	25,40,40	0.93	1 (4%)
4	VDO	B	1462	-	28,28,28	1.70	5 (17%)	31,42,42	1.52	7 (22%)
4	VDO	C	1458	-	28,28,28	1.57	6 (21%)	31,42,42	1.46	4 (12%)
2	EDO	A	1459	-	3,3,3	0.38	0	2,2,2	0.48	0
2	EDO	B	1459	-	3,3,3	0.41	0	2,2,2	0.35	0
3	UDP	D	1458	-	20,26,26	1.25	2 (10%)	25,40,40	1.08	1 (4%)
2	EDO	A	1457	-	3,3,3	0.66	0	2,2,2	0.19	0
3	UDP	B	1461	-	20,26,26	1.21	1 (5%)	25,40,40	1.08	1 (4%)
2	EDO	A	1458	-	3,3,3	0.70	0	2,2,2	0.33	0
4	VDO	A	1461	-	28,28,28	1.72	5 (17%)	31,42,42	1.37	3 (9%)

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	EDO	B	1460	-	-	0/1/1/1	-
4	VDO	D	1459	-	-	1/12/52/52	0/2/2/2
3	UDP	C	1457	-	-	5/14/32/32	0/2/2/2
3	UDP	A	1460	-	-	3/14/32/32	0/2/2/2
4	VDO	B	1462	-	-	0/12/52/52	0/2/2/2
4	VDO	C	1458	-	-	2/12/52/52	0/2/2/2
2	EDO	A	1459	-	-	0/1/1/1	-
2	EDO	B	1459	-	-	1/1/1/1	-
3	UDP	D	1458	-	-	3/14/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	1457	-	-	0/1/1/1	-
3	UDP	B	1461	-	-	3/14/32/32	0/2/2/2
2	EDO	A	1458	-	-	1/1/1/1	-
4	VDO	A	1461	-	-	3/12/52/52	0/2/2/2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1459	VDO	CAL-CAK	5.29	1.40	1.32
4	A	1461	VDO	CAL-CAK	5.15	1.40	1.32
4	B	1462	VDO	CAL-CAK	4.90	1.39	1.32
4	C	1458	VDO	CAL-CAK	4.61	1.39	1.32
4	B	1462	VDO	CAJ-CAM	4.43	1.58	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1462	VDO	CAF-CAV-CAA	4.10	113.63	108.49
4	C	1458	VDO	CAL-CAM-NAN	-3.73	105.09	110.68
4	C	1458	VDO	CAF-CAV-CAA	3.64	113.05	108.49
4	A	1461	VDO	CAF-CAV-CAA	3.58	112.97	108.49
4	B	1462	VDO	CAL-CAM-NAN	-3.32	105.69	110.68

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1458	VDO	OAQ-CAD-CAK-CAL
3	D	1458	UDP	PB-O3A-PA-O5'
3	C	1457	UDP	O4'-C1'-N1-C6
3	C	1457	UDP	PB-O3A-PA-O5'
3	C	1457	UDP	PA-O3A-PB-O2B

There are no ring outliers.

8 monomers are involved in 22 short contacts:

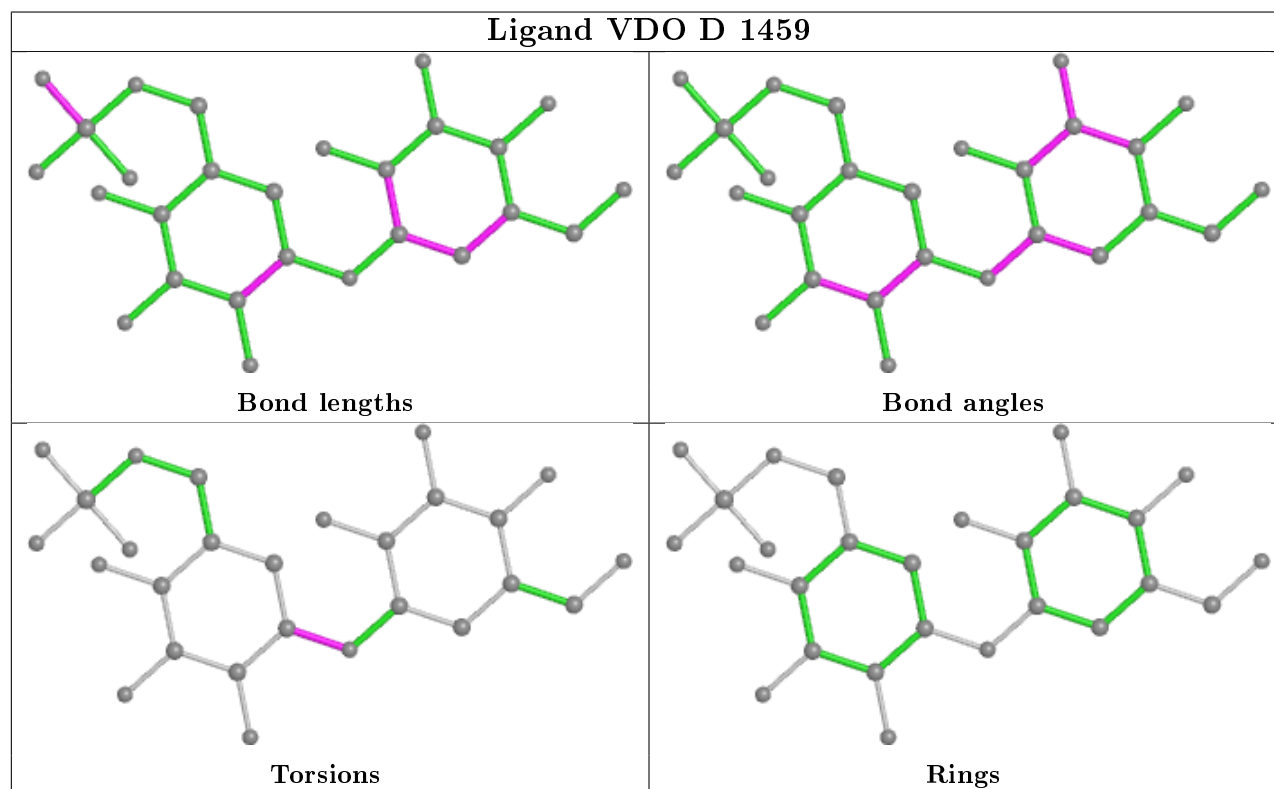
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1459	VDO	1	0
4	B	1462	VDO	3	0
4	C	1458	VDO	2	0

*Continued on next page...*

*Continued from previous page...*

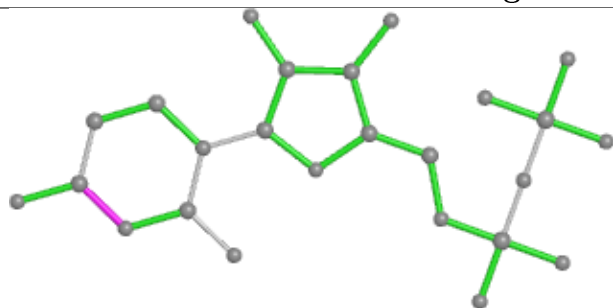
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1459	EDO	5	0
2	B	1459	EDO	4	0
3	B	1461	UDP	1	0
2	A	1458	EDO	4	0
4	A	1461	VDO	3	0

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.

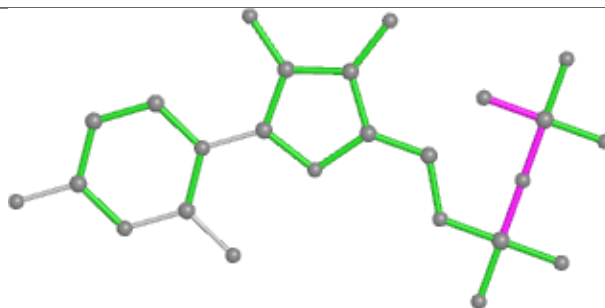




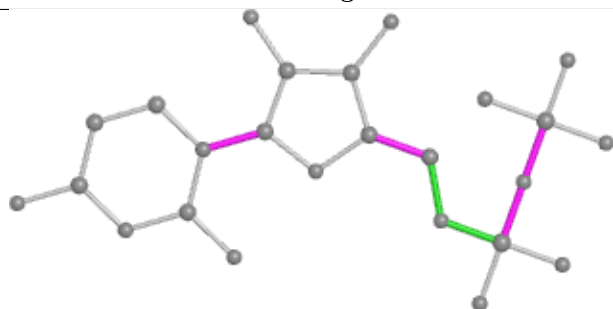
## Ligand UDP C 1457



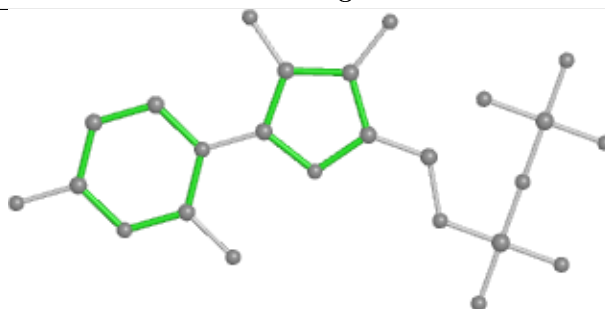
Bond lengths



Bond angles

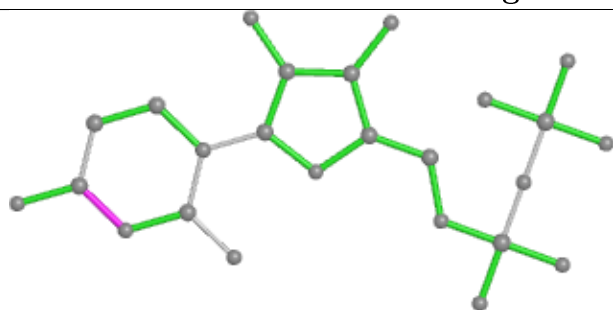


Torsions

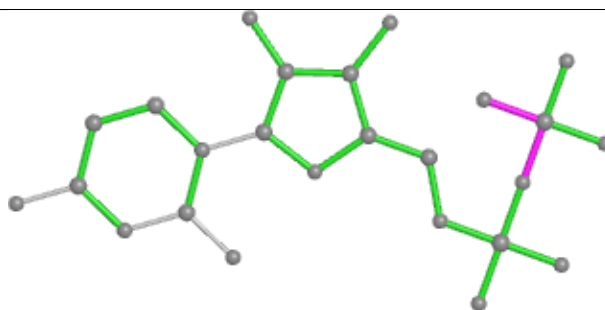


Rings

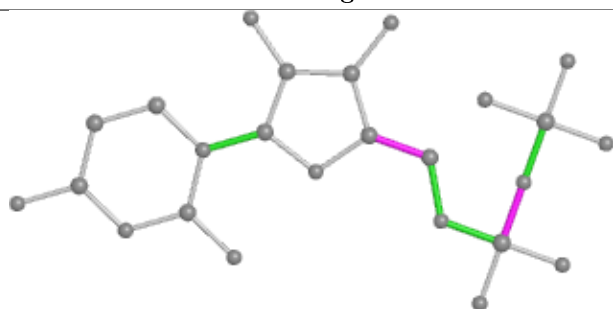
## Ligand UDP A 1460



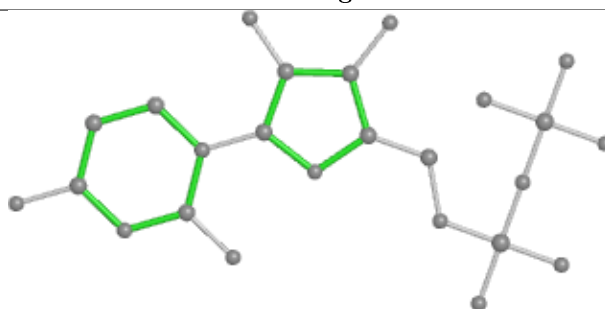
Bond lengths



Bond angles

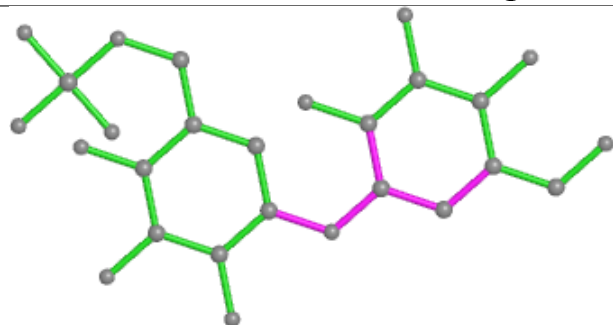


Torsions

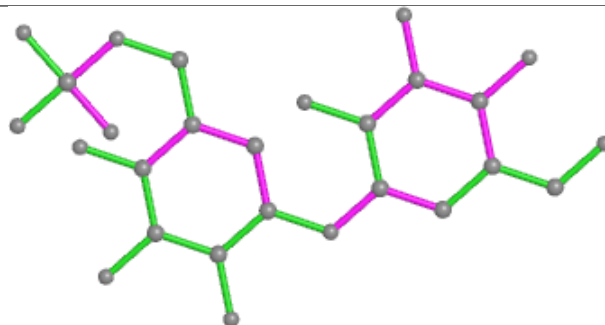


Rings

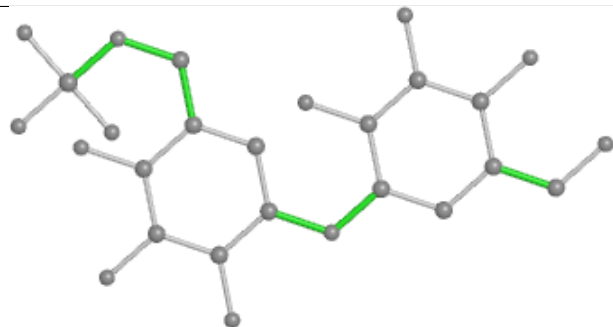
## Ligand VDO B 1462



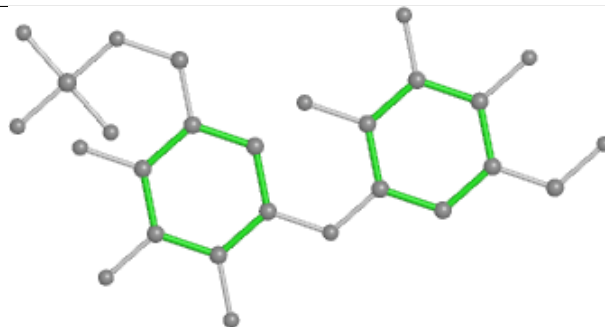
Bond lengths



Bond angles

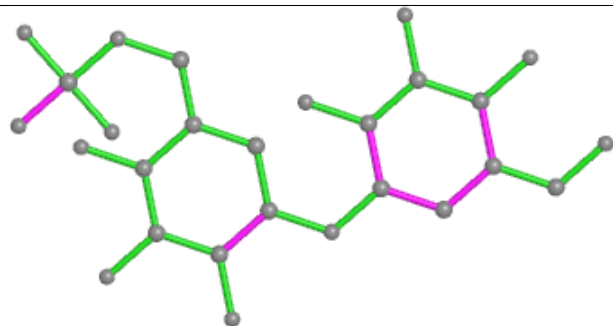


Torsions

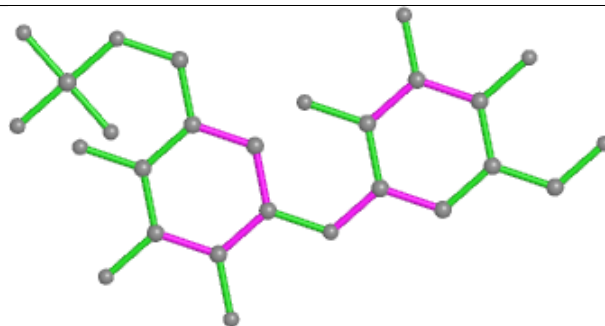


Rings

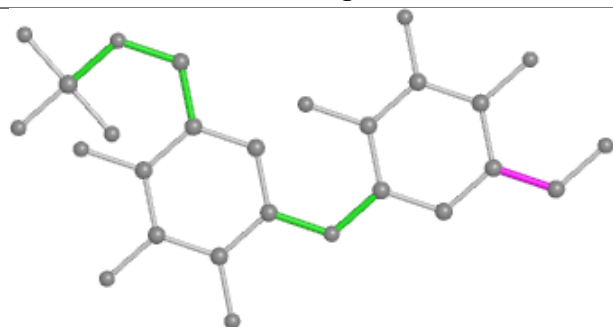
## Ligand VDO C 1458



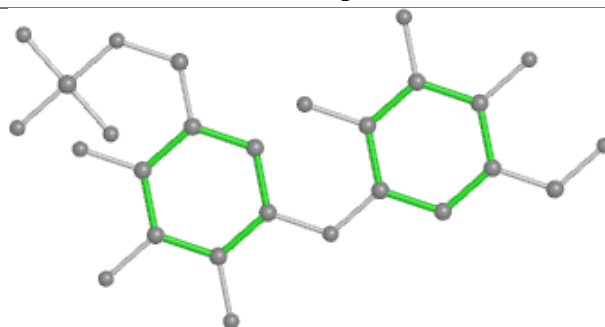
Bond lengths



Bond angles

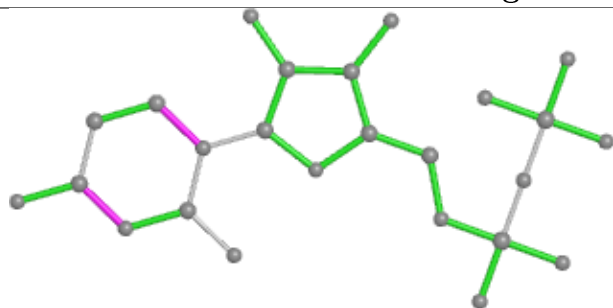


Torsions

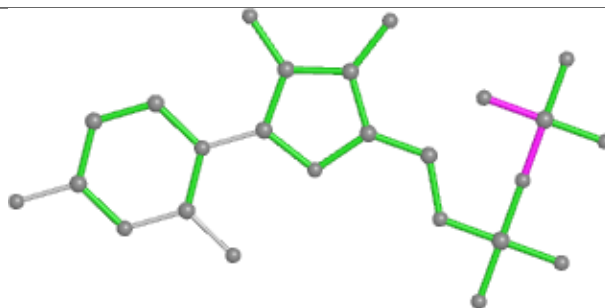


Rings

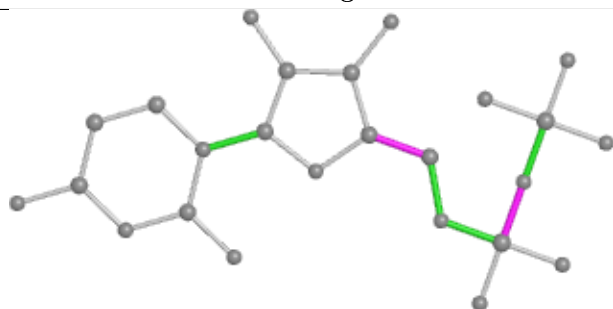
## Ligand UDP D 1458



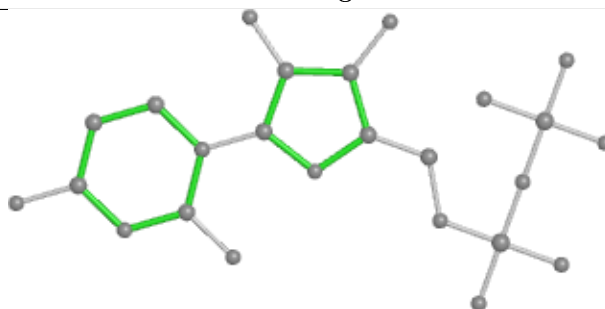
Bond lengths



Bond angles

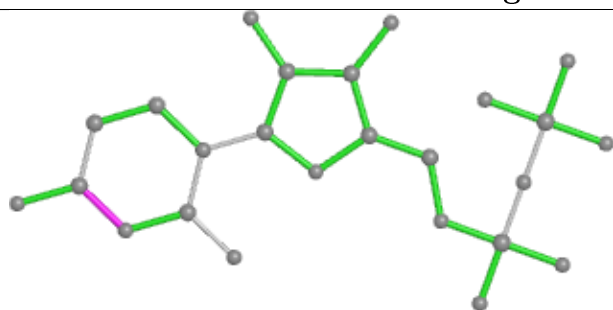


Torsions

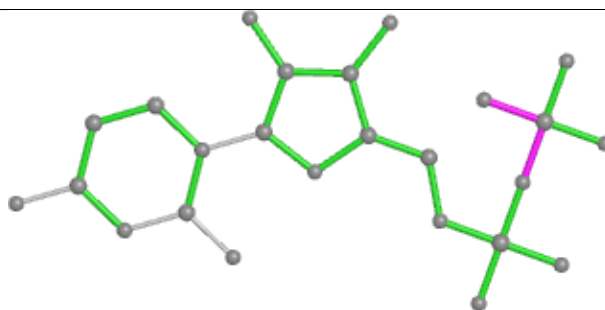


Rings

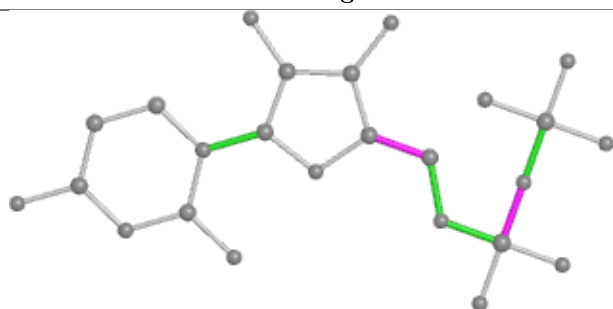
## Ligand UDP B 1461



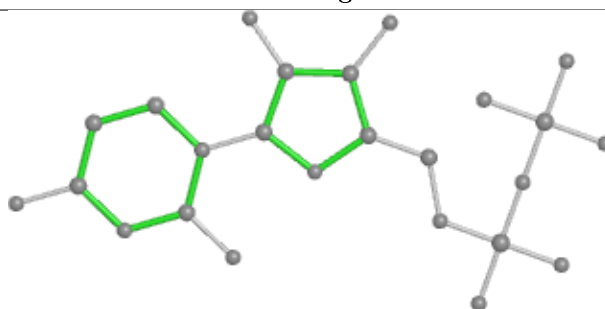
Bond lengths



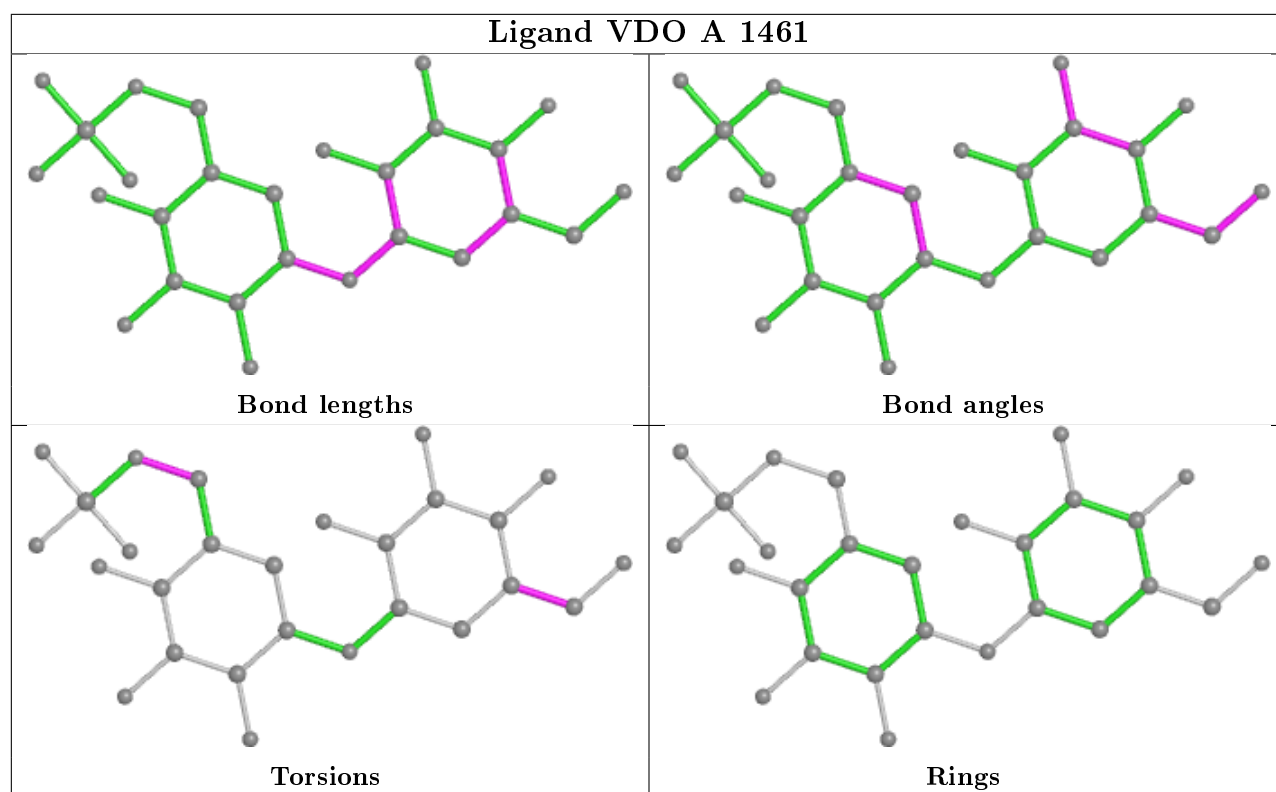
Bond angles



Torsions



Rings



## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	456/474 (96%)	-0.40	2 (0%) 92 91	9, 19, 39, 63	0
1	B	454/474 (95%)	-0.22	4 (0%) 84 83	11, 26, 53, 65	0
1	C	440/474 (92%)	0.24	22 (5%) 28 27	20, 37, 76, 88	0
1	D	457/474 (96%)	-0.29	3 (0%) 87 86	13, 25, 48, 62	0
All	All	1807/1896 (95%)	-0.17	31 (1%) 70 68	9, 26, 62, 88	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	206	ARG	5.8
1	C	52	LEU	5.0
1	C	251	LEU	4.2
1	C	36	GLY	4.1
1	C	53	LYS	3.9

### 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](#)

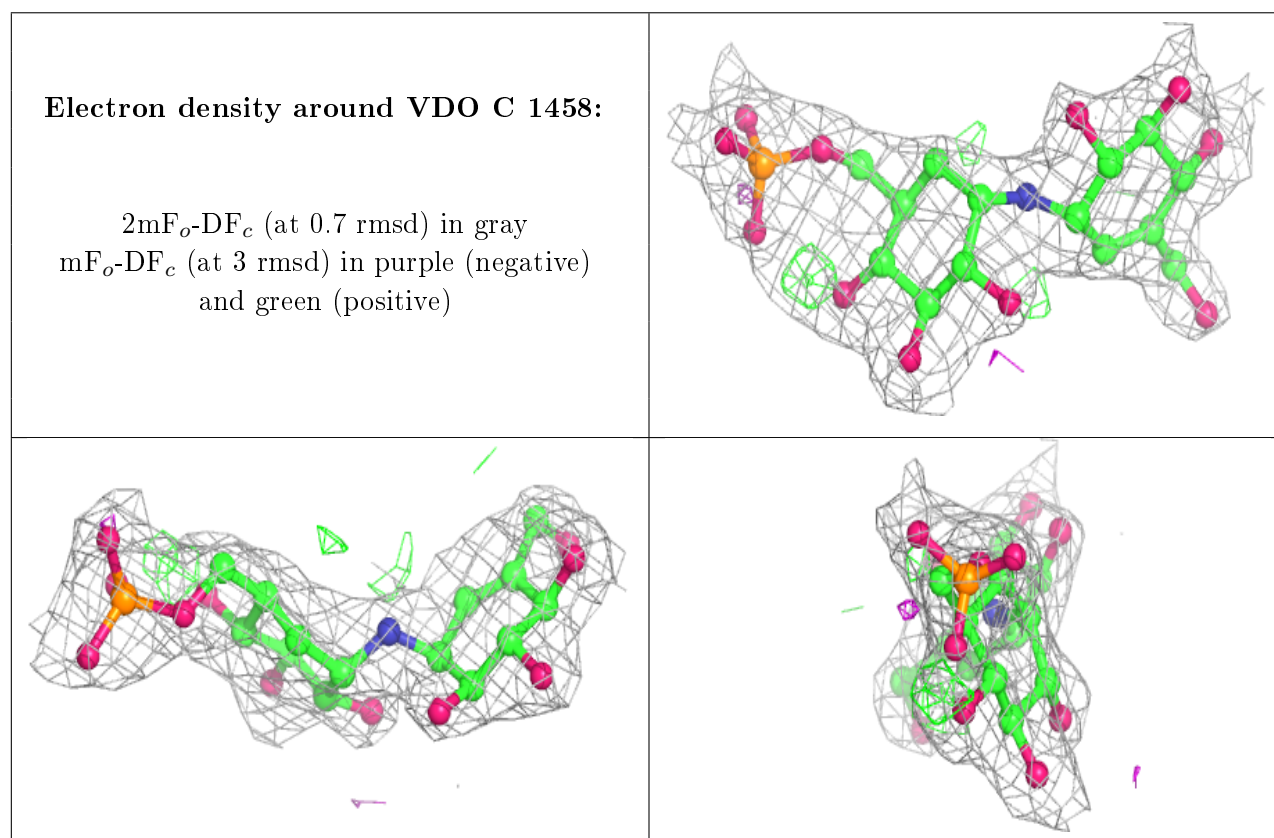
There are no carbohydrates in this entry.

### 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, 95<sup>th</sup> 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.

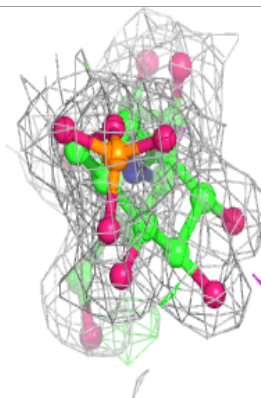
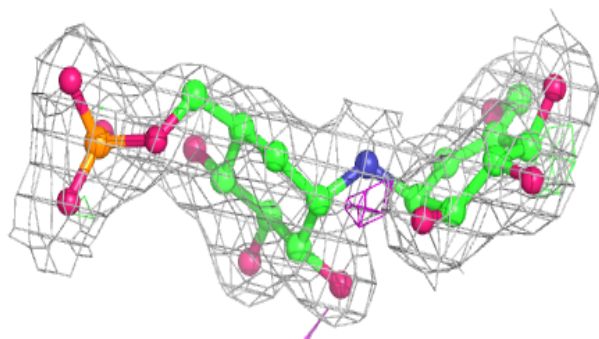
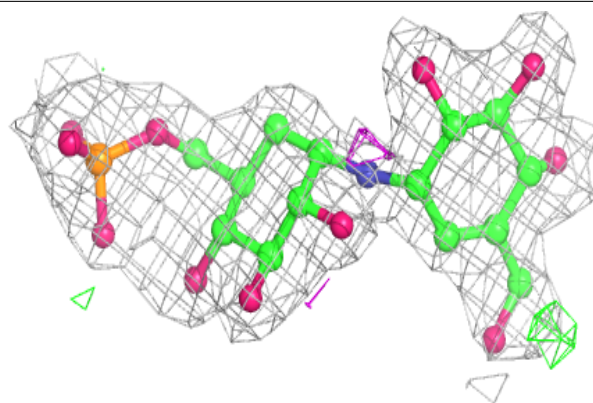
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	A	1458	4/4	0.71	0.47	33,40,40,43	0
2	EDO	A	1457	4/4	0.82	0.21	35,36,37,37	0
2	EDO	B	1460	4/4	0.88	0.27	33,37,38,40	0
4	VDO	C	1458	27/27	0.92	0.13	35,40,42,44	0
2	EDO	A	1459	4/4	0.93	0.28	23,25,25,29	0
4	VDO	B	1462	27/27	0.94	0.12	15,23,31,32	0
4	VDO	D	1459	27/27	0.95	0.11	15,23,28,30	0
2	EDO	B	1459	4/4	0.95	0.25	25,30,30,32	0
4	VDO	A	1461	27/27	0.95	0.13	13,17,20,27	0
3	UDP	C	1457	25/25	0.97	0.11	31,37,38,39	0
3	UDP	D	1458	25/25	0.98	0.10	16,20,24,25	0
3	UDP	A	1460	25/25	0.99	0.10	12,15,17,19	0
3	UDP	B	1461	25/25	0.99	0.10	16,25,28,28	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.

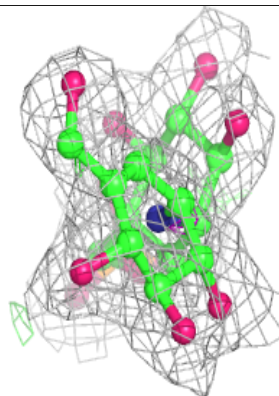
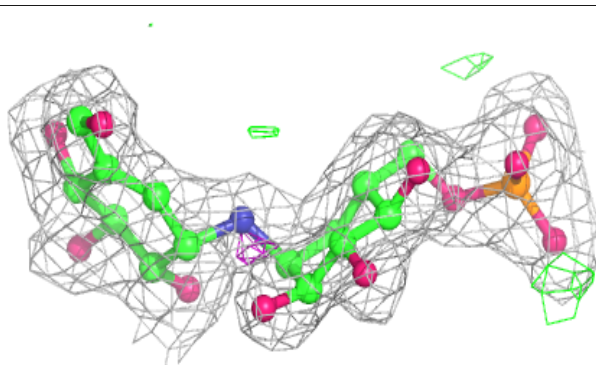
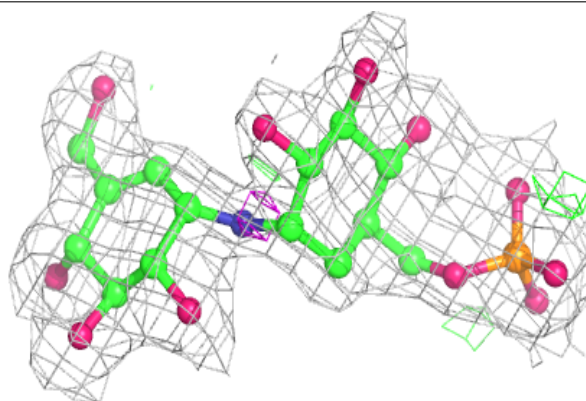


**Electron density around VDO B 1462:**

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

**Electron density around VDO D 1459:**

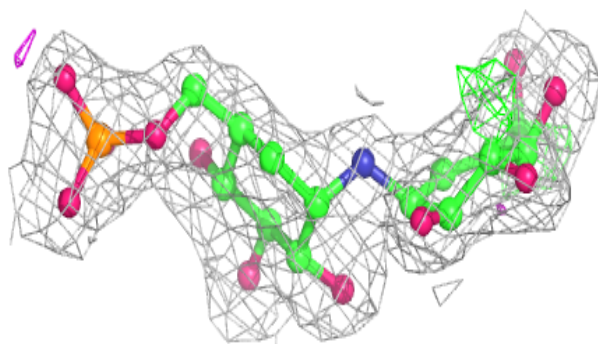
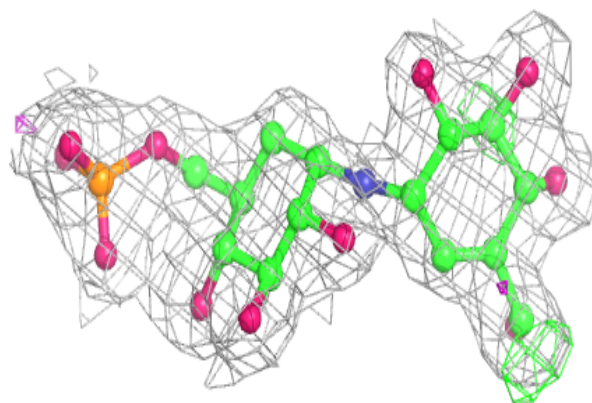
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



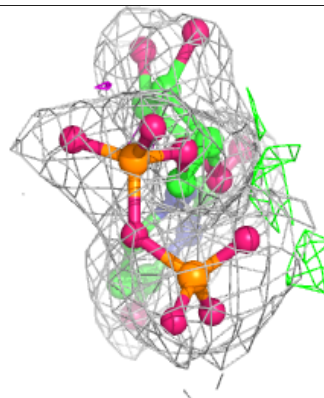
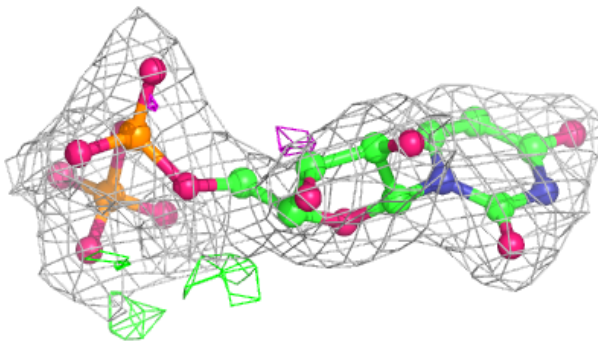
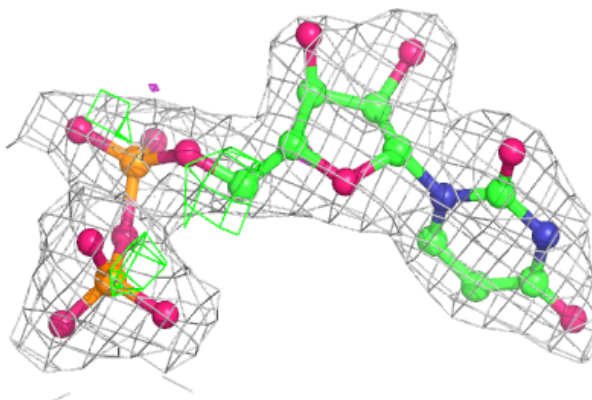


**Electron density around VDO A 1461:**

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

**Electron density around UDP C 1457:**

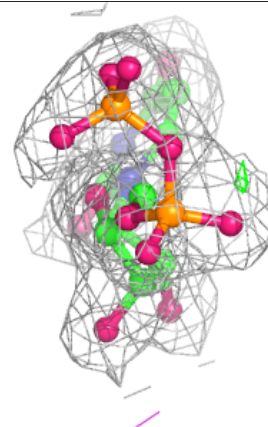
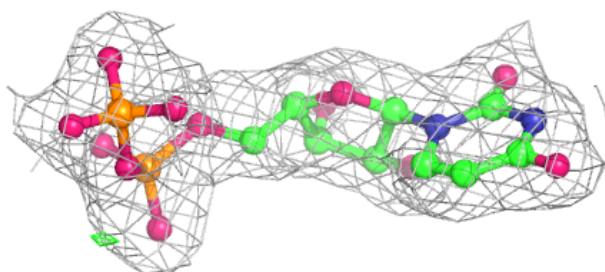
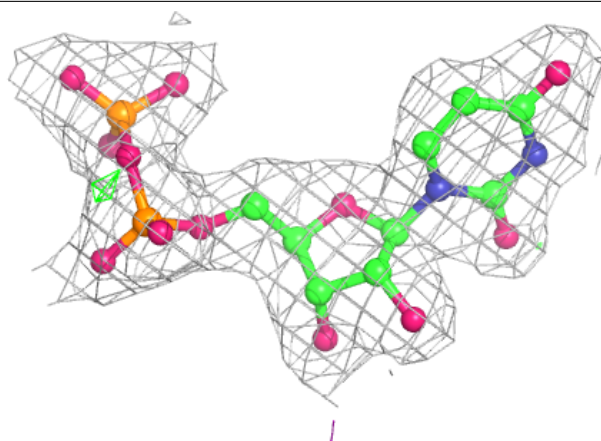
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



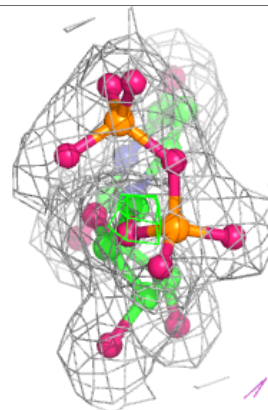
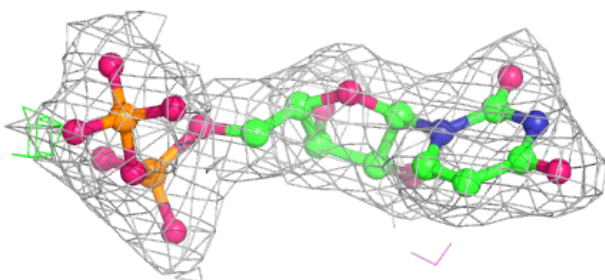
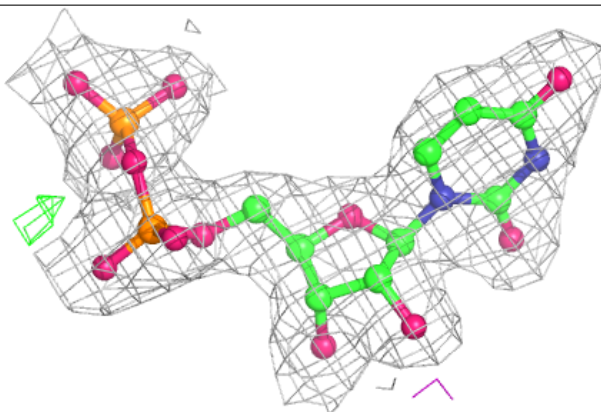


**Electron density around UDP D 1458:**

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

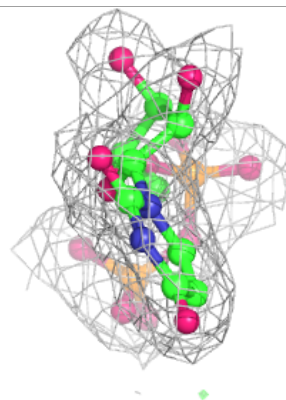
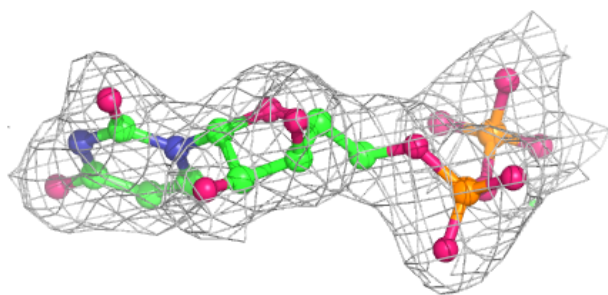
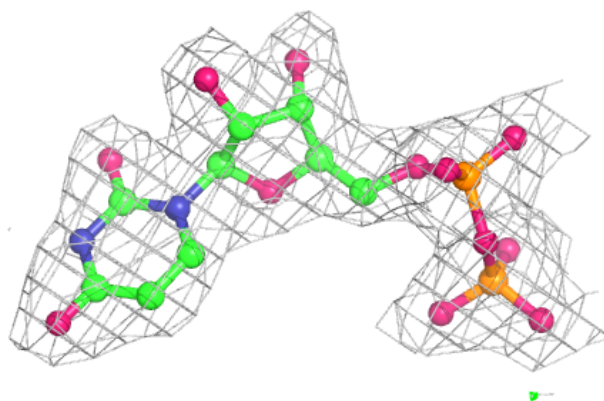
**Electron density around UDP A 1460:**

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



**Electron density around UDP B 1461:**

$2mF_o-DF_c$  (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.