W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 05:58 pm BST

PDB ID	:	5VR8
Title	:	Human UDP-Glucose Dehydrogenase with UDP-Xylose Bound to the Co-enzyme Site
Authors	:	Kadirvelraj, R.; Beattie, N.R.; Wood, Z.A.
Deposited on	:	2017-05-10
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

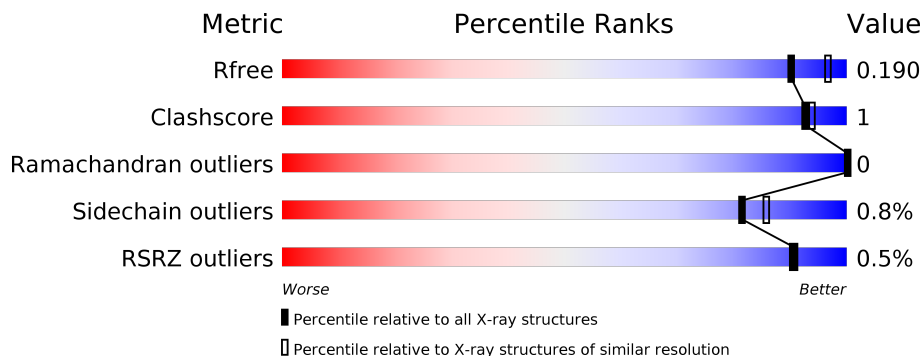|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Percentile Ranks	Value
Rfree		0.190
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		0.8%
RSRZ outliers		0.5%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 >=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	A	495	88% • 7%
1	B	495	87% 5% • 7%
1	C	495	% 89% • 7%
1	D	495	89% • 8%
1	E	495	91% • 8%
1	F	495	% 89% • 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23064 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 UDP-glucose 6-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3607	2281	623	683	20			
1	B	459	Total	C	N	O	S	0	0	0
			3599	2277	622	680	20			
1	C	462	Total	C	N	O	S	0	0	0
			3626	2292	627	687	20			
1	D	457	Total	C	N	O	S	0	0	0
			3581	2266	618	678	19			
1	E	457	Total	C	N	O	S	0	0	0
			3581	2266	618	678	19			
1	F	458	Total	C	N	O	S	0	0	0
			3589	2271	619	679	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP O60701
B	0	HIS	-	expression tag	UNP O60701
C	0	HIS	-	expression tag	UNP O60701
D	0	HIS	-	expression tag	UNP O60701
E	0	HIS	-	expression tag	UNP O60701
F	0	HIS	-	expression tag	UNP O60701

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-XYLOPYRANOSE (three-letter code: UDX) (formula: $C_{14}H_{22}N_2O_{16}P_2$).
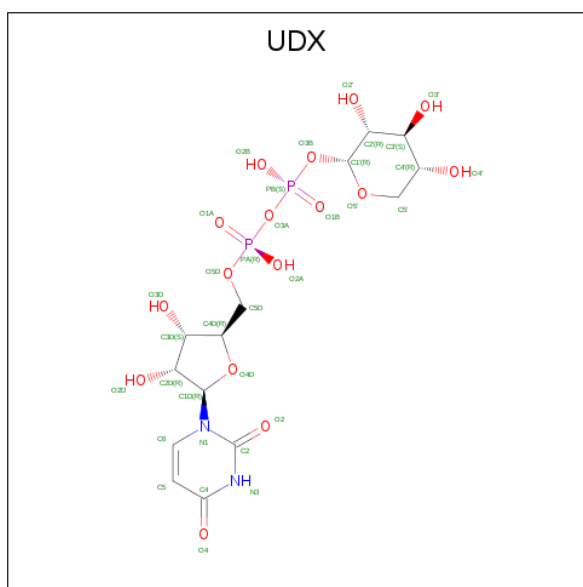
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	A	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	B	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	B	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	C	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	D	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	D	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	E	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	E	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	F	1	Total	C	N	O	P	0	0
			34	14	2	16	2		

- Molecule 3 is A D E N O S I N E - 5'- D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
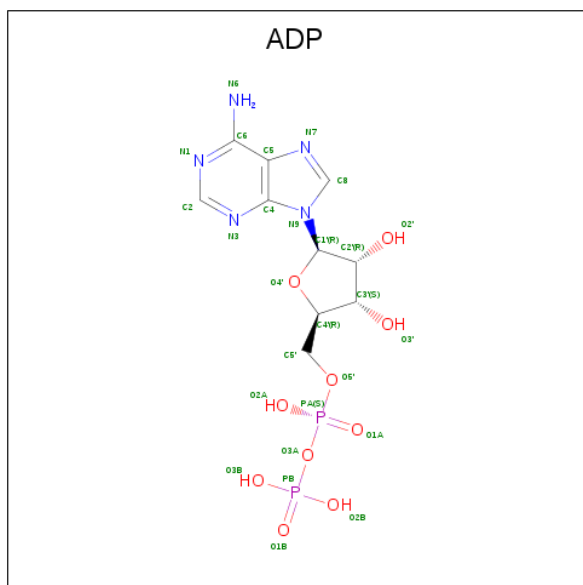
ADP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	233	Total	O	0	0
			233	233		
4	C	188	Total	O	0	0
			188	188		
4	D	209	Total	O	0	0
			209	209		
4	E	138	Total	O	0	0
			138	138		
4	F	126	Total	O	0	0
			126	126		

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: UDP-glucose 6-dehydrogenase
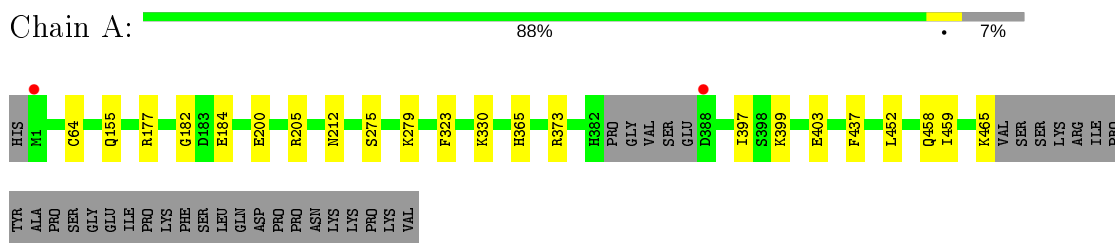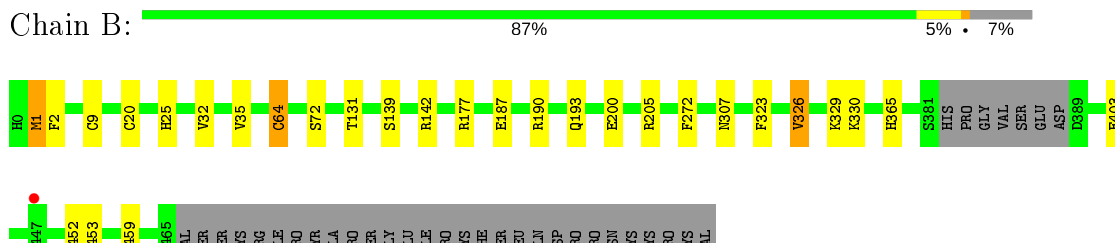
Chain A:

- Molecule 1: UDP-glucose 6-dehydrogenase

Chain B:

- Molecule 1: UDP-glucose 6-dehydrogenase
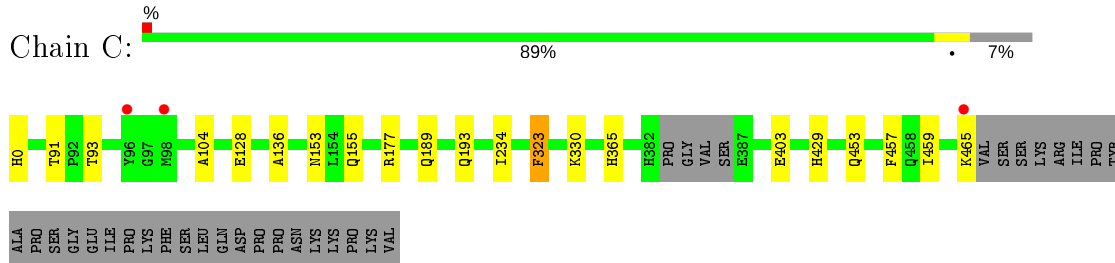
Chain C:

- Molecule 1: UDP-glucose 6-dehydrogenase
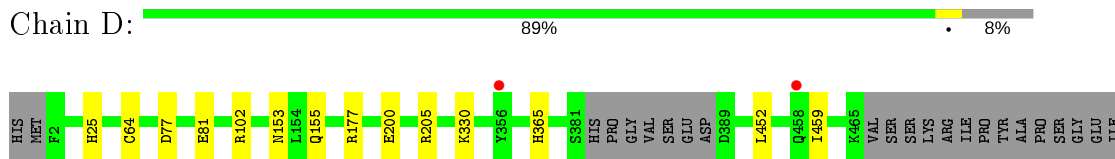
Chain D:

PRO LYS PHE SER LEU GLN ASP PRO PRO ASN LYS LYS PRO LYS VAL
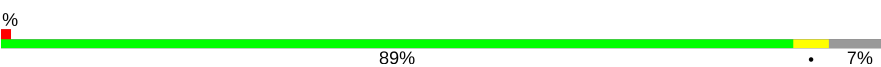
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain E:

91%   •   8%

HIS MET F2 C64 N153 L154 Q155 R177 K267 F323 K330 H365 S381 HIS PRO GLY VAL SER GLU ASP D389 G447 K465 VAL SER SER LYS ARG ILE PRO TYR ALA PRO SER GLY GLU ILE PRO LYS PHE SER LEU GLN ASP PRO PRO ASN LYS LYS PRO

LYS VAL

• Molecule 1: UDP-glucose 6-dehydrogenase

%

Chain F:

89%   •   7%

HIS M1 V37 T91 P92 T93 Y96 G97 M98 G101 A104 Y108 E128 A136 R177 Q193 F323 K330 H365 R373 S381 HIS PRO GLY VAL SER GLU ASP D389 I397 F437 D446 Q458 I459 K465 VAL SER SER LYS ARG

ILE PRO TYR ALA PRO SER GLY GLU ILE PRO LYS PHE SER LEU GLN ASP PRO PRO ASN LYS LYS PRO LYS VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.08Å 196.49Å 111.26Å 90.00° 111.91° 90.00°	Depositor
Resolution (Å)	49.12 – 2.00 91.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.12-2.00) 93.3 (91.38-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.156 , 0.190 0.156 , 0.190	Depositor DCC
R_{free} test set	11196 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23064	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UDX, ADP

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	0.43	1/3672 (0.0%)	0.55	0/4967
1	B	0.44	1/3664 (0.0%)	0.55	0/4956
1	C	0.41	0/3692	0.55	0/4994
1	D	0.40	1/3645 (0.0%)	0.52	0/4931
1	E	0.37	1/3645 (0.0%)	0.51	0/4931
1	F	0.36	0/3653	0.51	0/4941
All	All	0.40	4/21971 (0.0%)	0.53	0/29720

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	64	CYS	CB-SG	-7.57	1.69	1.82
1	B	64	CYS	CB-SG	-7.31	1.69	1.82
1	E	64	CYS	CB-SG	-6.13	1.71	1.82
1	A	64	CYS	CB-SG	-5.54	1.72	1.81

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	3607	0	3622	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3599	0	3618	20	0
1	C	3626	0	3635	14	0
1	D	3581	0	3599	8	0
1	E	3581	0	3599	3	0
1	F	3589	0	3611	11	0
2	A	68	0	40	0	0
2	B	68	0	40	1	0
2	C	34	0	20	0	0
2	D	68	0	40	0	0
2	E	68	0	40	0	0
2	F	34	0	20	0	0
3	C	27	0	12	0	0
3	F	27	0	12	1	0
4	A	193	0	0	3	0
4	B	233	0	0	1	0
4	C	188	0	0	2	0
4	D	209	0	0	2	0
4	E	138	0	0	0	0
4	F	126	0	0	1	0
All	All	23064	0	21908	65	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.

The worst 5 of 65 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:B:187:GLU:OE2	1:B:190:ARG:NH2	2.19	0.74
1:B:452:LEU:HB2	1:B:459:ILE:HD11	1.76	0.68
1:B:272:PHE:H	1:B:307:ASN:HD21	1.42	0.68
1:E:153:ASN:OD1	1:E:155:GLN:NE2	2.27	0.67
1:F:91:THR:CG2	1:F:104:ALA:HB1	2.28	0.64

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	456/495 (92%)	446 (98%)	10 (2%)	0	100	100
1	B	455/495 (92%)	445 (98%)	10 (2%)	0	100	100
1	C	458/495 (92%)	447 (98%)	11 (2%)	0	100	100
1	D	453/495 (92%)	443 (98%)	10 (2%)	0	100	100
1	E	453/495 (92%)	443 (98%)	10 (2%)	0	100	100
1	F	454/495 (92%)	444 (98%)	10 (2%)	0	100	100
All	All	2729/2970 (92%)	2668 (98%)	61 (2%)	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	A	395/427 (92%)	392 (99%)	3 (1%)	81	86
1	B	394/427 (92%)	389 (99%)	5 (1%)	69	74
1	C	397/427 (93%)	392 (99%)	5 (1%)	69	74
1	D	392/427 (92%)	391 (100%)	1 (0%)	92	95
1	E	392/427 (92%)	390 (100%)	2 (0%)	88	92
1	F	393/427 (92%)	389 (99%)	4 (1%)	76	81
All	All	2363/2562 (92%)	2343 (99%)	20 (1%)	81	86

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	93	THR
1	C	177	ARG
1	F	177	ARG
1	B	326	VAL
1	C	0	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	118	GLN
1	D	159	ASN
1	F	155	GLN
1	C	301	GLN
1	F	25	HIS

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 ⓘ

12 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	UDX	D	501	-	29,36,36	0.74	0	38,55,55	1.15	2 (5%)
2	UDX	A	501	-	29,36,36	0.81	1 (3%)	38,55,55	1.03	2 (5%)
2	UDX	B	501	-	29,36,36	0.80	1 (3%)	38,55,55	1.08	2 (5%)
2	UDX	B	502	-	29,36,36	0.76	1 (3%)	38,55,55	1.06	3 (7%)
2	UDX	D	502	-	29,36,36	0.88	2 (6%)	38,55,55	0.97	1 (2%)
3	ADP	C	500	-	24,29,29	1.01	2 (8%)	29,45,45	1.27	3 (10%)
3	ADP	F	500	-	24,29,29	1.06	2 (8%)	29,45,45	1.27	2 (6%)
2	UDX	E	502	-	29,36,36	0.79	2 (6%)	38,55,55	0.86	1 (2%)
2	UDX	C	501	-	29,36,36	0.79	1 (3%)	38,55,55	0.99	2 (5%)
2	UDX	A	502	-	29,36,36	0.64	0	38,55,55	0.84	2 (5%)
2	UDX	E	501	-	29,36,36	0.85	2 (6%)	38,55,55	0.98	2 (5%)
2	UDX	F	501	-	29,36,36	0.75	0	38,55,55	0.76	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
2	UDX	D	501	-	-	6/19/54/54	0/3/3/3
2	UDX	A	501	-	-	6/19/54/54	0/3/3/3
2	UDX	B	501	-	-	6/19/54/54	0/3/3/3
2	UDX	B	502	-	-	3/19/54/54	0/3/3/3
2	UDX	D	502	-	-	2/19/54/54	0/3/3/3
3	ADP	C	500	-	-	1/12/32/32	0/3/3/3
3	ADP	F	500	-	-	1/12/32/32	0/3/3/3
2	UDX	E	502	-	-	1/19/54/54	0/3/3/3
2	UDX	C	501	-	-	3/19/54/54	0/3/3/3
2	UDX	A	502	-	-	3/19/54/54	0/3/3/3
2	UDX	E	501	-	-	5/19/54/54	0/3/3/3
2	UDX	F	501	-	-	1/19/54/54	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	UDX	O4D-C1D	3.02	1.45	1.41
3	F	500	ADP	C5-C4	2.55	1.47	1.40
3	C	500	ADP	C5-C4	2.53	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	500	ADP	C2-N3	2.24	1.35	1.32
3	C	500	ADP	C2-N3	2.24	1.35	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	UDX	O3B-C1'-C2'	3.90	115.53	108.38
2	B	502	UDX	O3A-PB-O3B	3.13	108.79	102.48
3	F	500	ADP	N3-C2-N1	-3.05	123.92	128.68
3	F	500	ADP	C4-C5-N7	-3.04	106.23	109.40
3	C	500	ADP	N3-C2-N1	-2.94	124.08	128.68

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	UDX	C1'-O3B-PB-O2B
2	D	501	UDX	O4D-C1D-N1-C6
2	D	501	UDX	C2D-C1D-N1-C6
2	A	501	UDX	C1'-O3B-PB-O2B
2	A	501	UDX	O4D-C1D-N1-C6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	UDX	1	0
3	F	500	ADP	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.

Ligand UDX D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand UDX A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand UDX B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand UDX B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand UDX D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 500

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP F 500

Bond lengths

Bond angles

Torsions

Rings

Ligand UDX E 502

Bond lengths

Bond angles

Torsions

Rings

Ligand UDX C 501	
Bond lengths	Bond angles
Torsions	Rings

Ligand UDX A 502	
Bond lengths	Bond angles
Torsions	Rings

Ligand UDX E 501

Bond lengths

Bond angles

Torsions

Rings

Ligand UDX F 501

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, 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	460/495 (92%)	-0.29	2 (0%)	92	92	16, 27, 47, 84	0
1	B	459/495 (92%)	-0.28	1 (0%)	95	94	15, 25, 45, 61	0
1	C	462/495 (93%)	-0.22	3 (0%)	89	88	17, 27, 53, 105	0
1	D	457/495 (92%)	-0.16	2 (0%)	92	92	19, 29, 63, 87	0
1	E	457/495 (92%)	-0.13	2 (0%)	92	92	18, 34, 67, 90	0
1	F	458/495 (92%)	-0.16	4 (0%)	84	83	19, 35, 57, 117	0
All	All	2753/2970 (92%)	-0.20	14 (0%)	91	90	15, 29, 57, 117	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	98	MET	5.6
1	C	98	MET	4.6
1	C	465	LYS	3.8
1	D	356	TYR	3.1
1	E	447	GLY	3.1

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, 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
2	UDX	E	501	34/34	0.96	0.13	27,36,54,56	0
2	UDX	A	501	34/34	0.97	0.12	22,30,47,48	0
2	UDX	B	501	34/34	0.97	0.13	18,26,44,46	0
3	ADP	F	500	27/27	0.97	0.10	31,39,47,54	0
2	UDX	D	501	34/34	0.97	0.12	19,29,51,52	0
2	UDX	E	502	34/34	0.98	0.10	18,22,25,29	0
3	ADP	C	500	27/27	0.98	0.10	24,29,43,46	0
2	UDX	F	501	34/34	0.98	0.09	19,22,26,28	0
2	UDX	C	501	34/34	0.99	0.10	15,18,22,23	0
2	UDX	A	502	34/34	0.99	0.10	15,19,21,23	0
2	UDX	D	502	34/34	0.99	0.10	17,22,24,27	0
2	UDX	B	502	34/34	0.99	0.09	14,17,19,20	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 UDX E 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
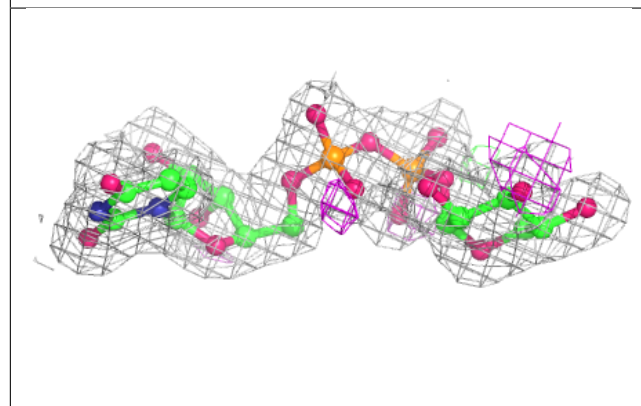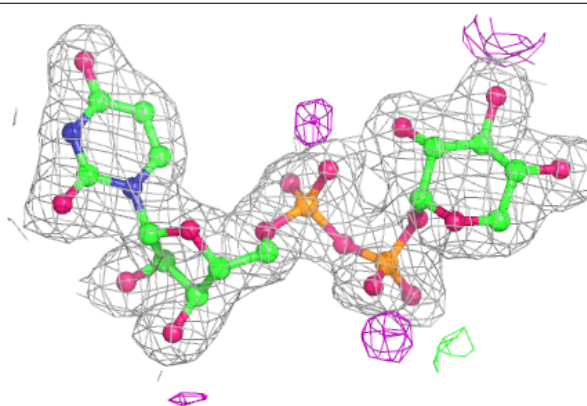and green (positive)
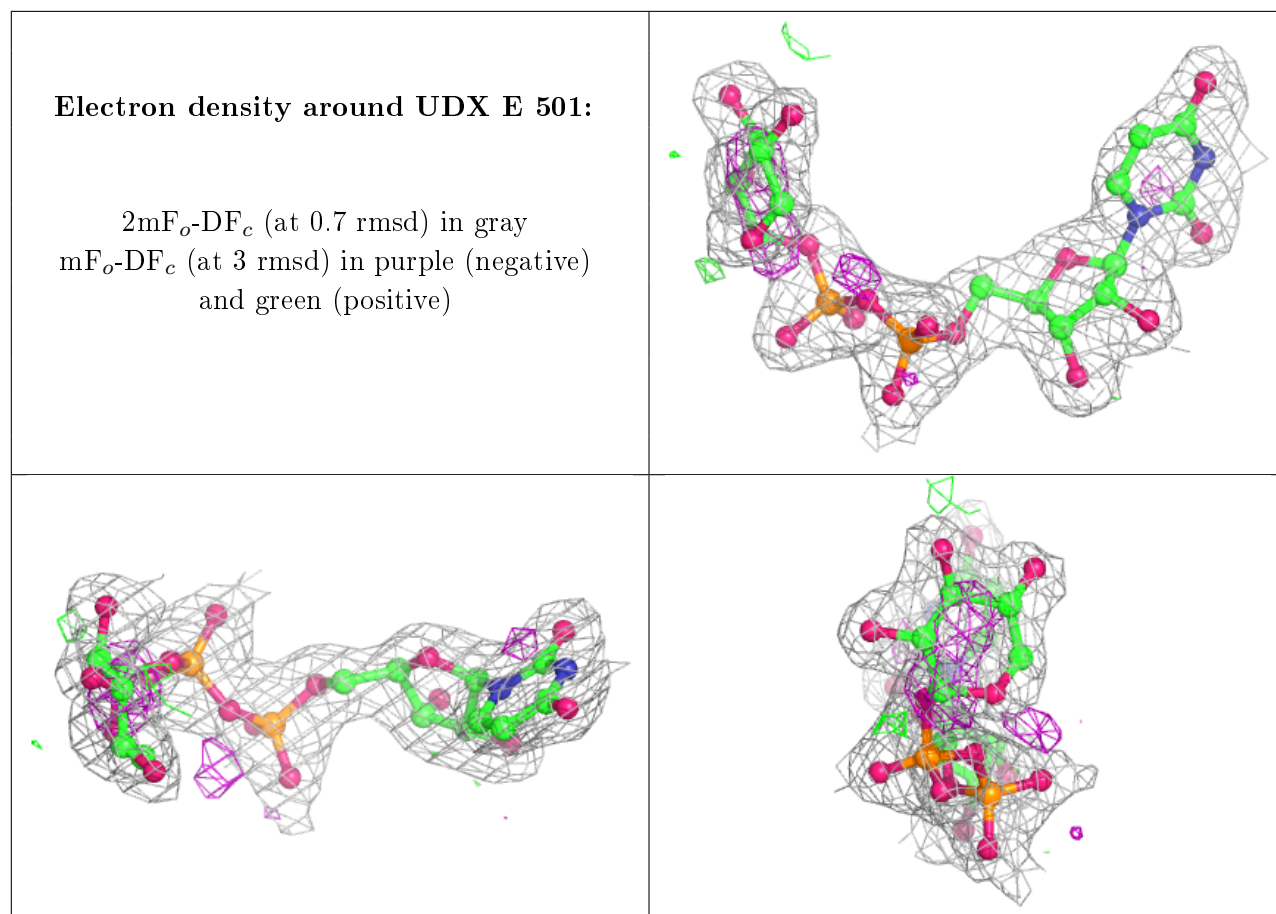
Electron density around UDX A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
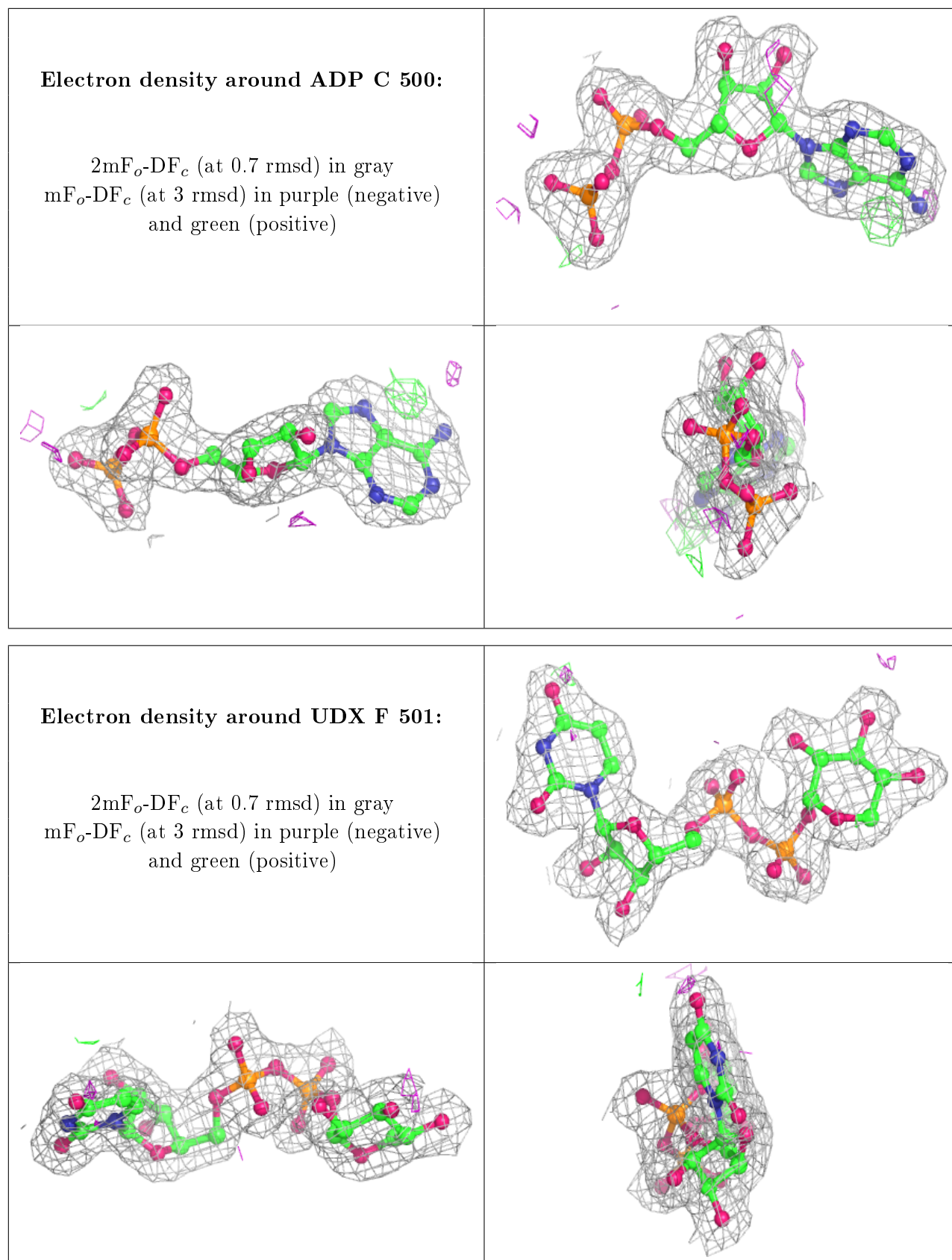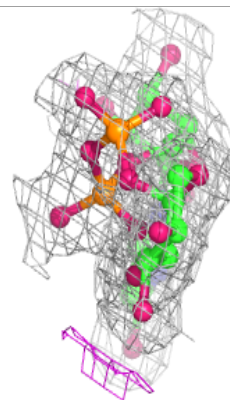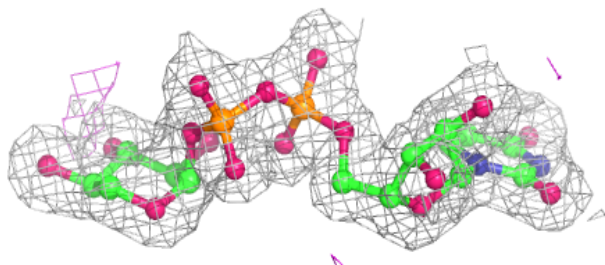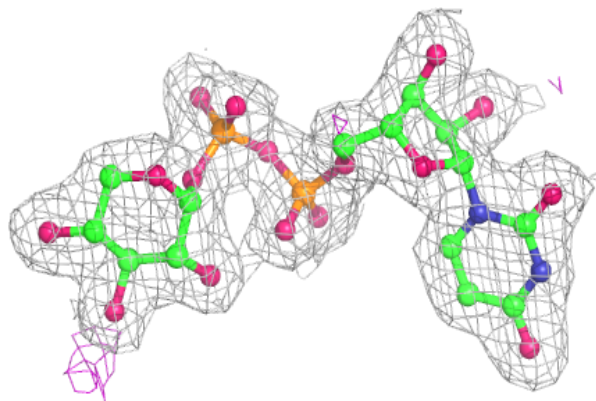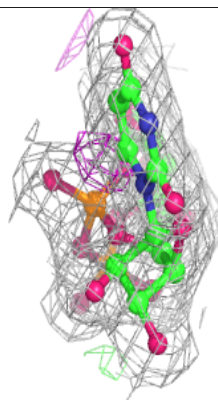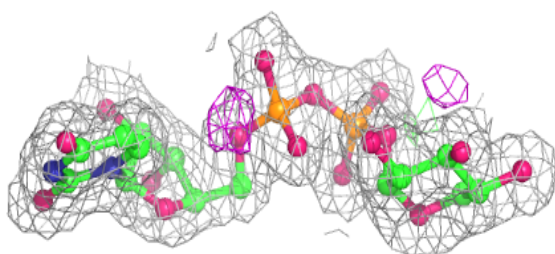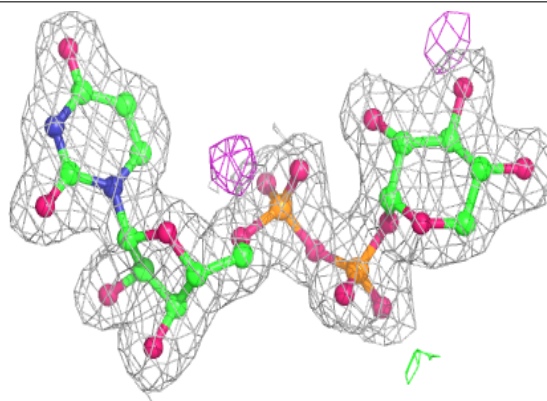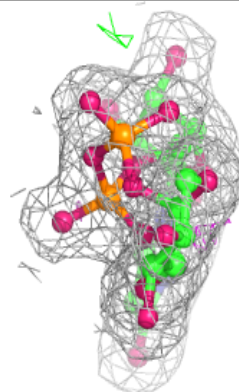mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
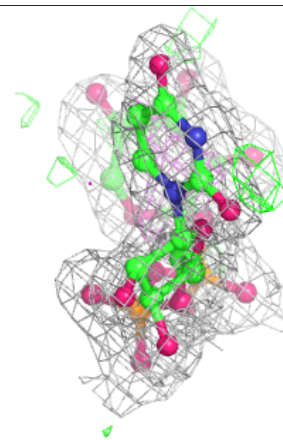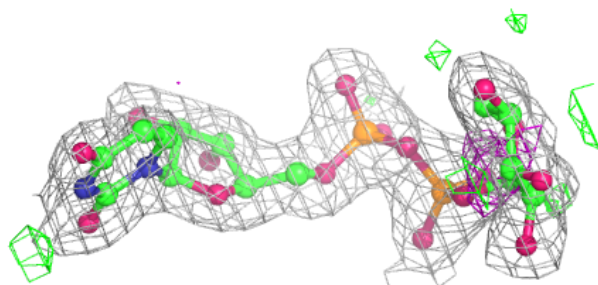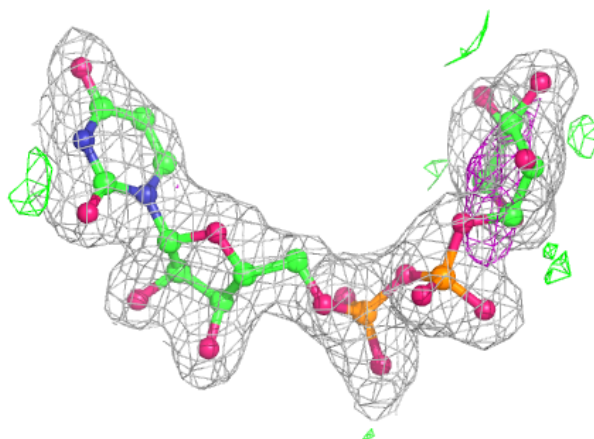
Electron density around UDX B 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
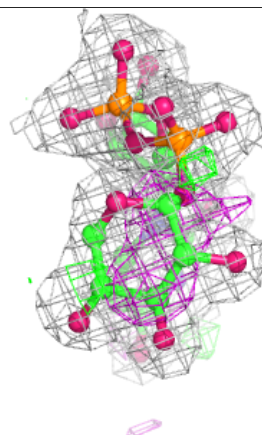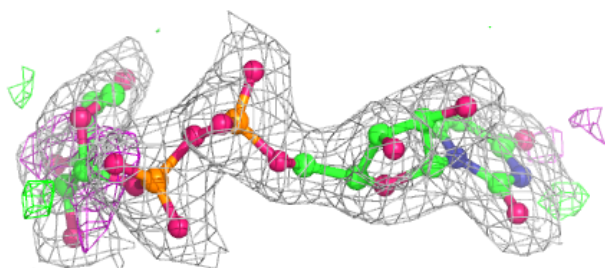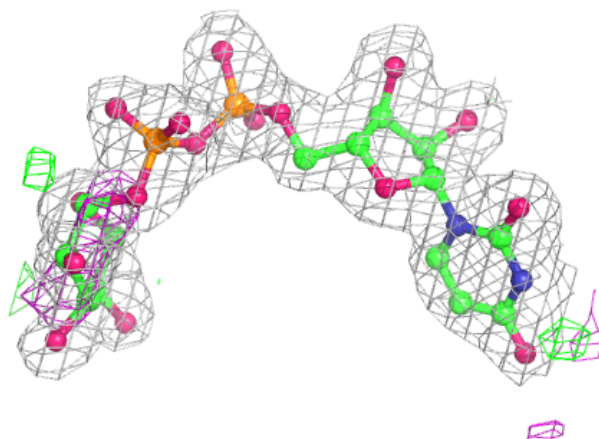
Electron density around ADP F 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
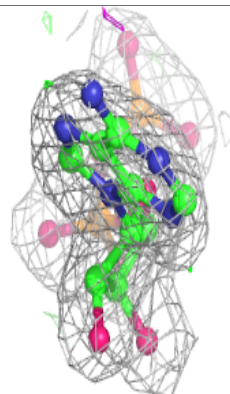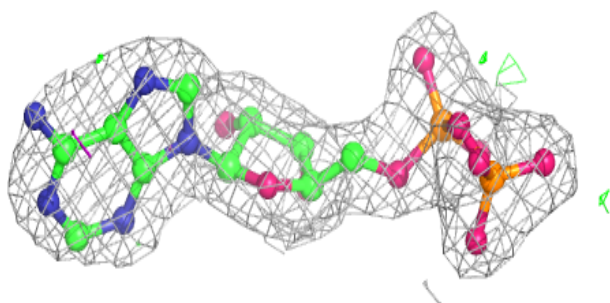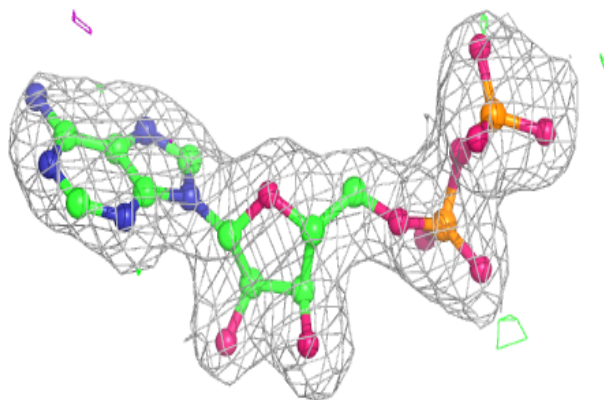
Electron density around UDX D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
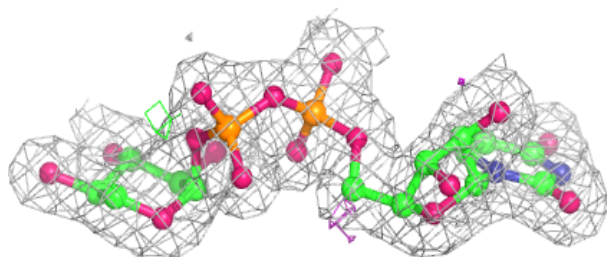mF_o-DF_c (at 3 rmsd) in purple (negative)
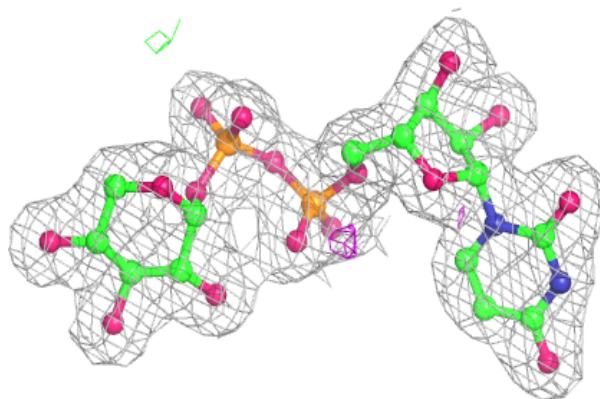and green (positive)
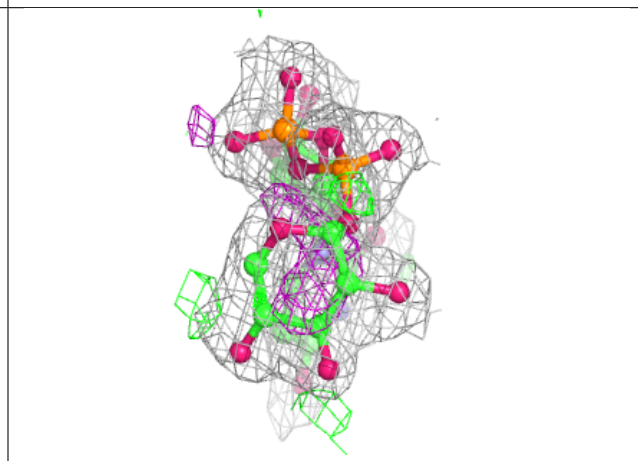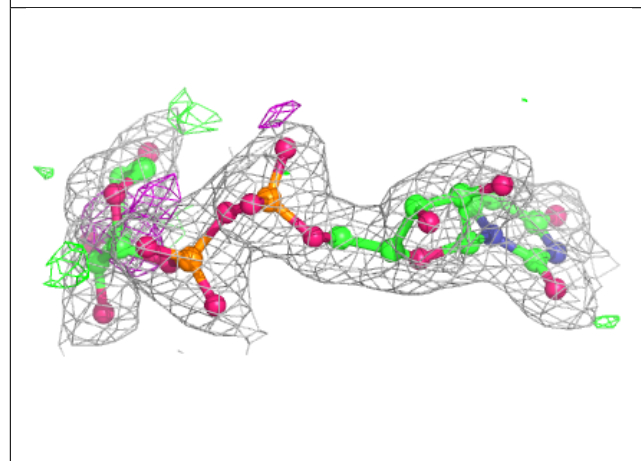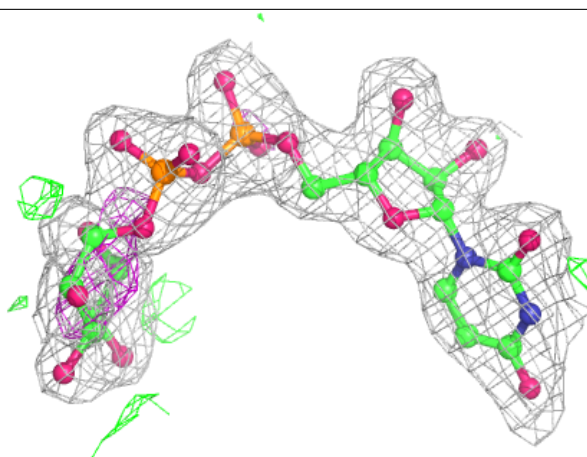
Electron density around UDX E 502:

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

Electron density around ADP C 500:

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

Electron density around UDX F 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
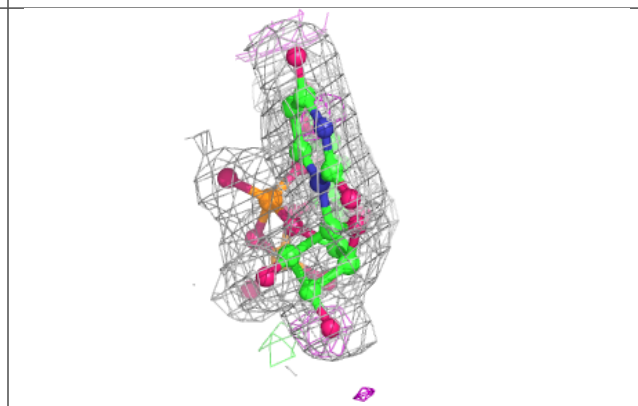
Electron density around UDX C 501:

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

Electron density around UDX A 502:

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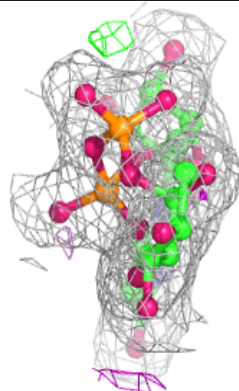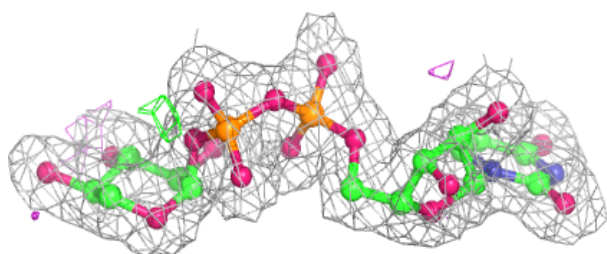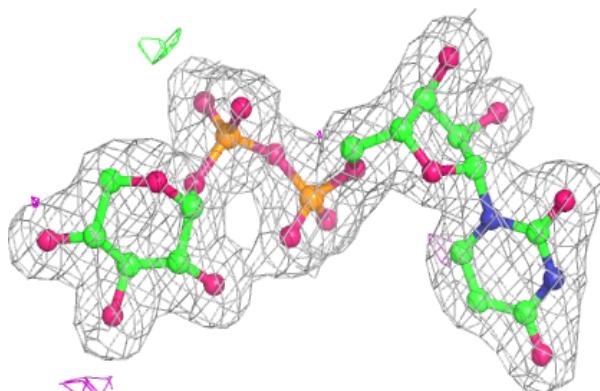mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around UDX D 502:

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

Electron density around UDX B 502:

$2mF_o-DF_c$ (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.