



Full wwPDB X-ray Structure Validation Report ⓘ

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)

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 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

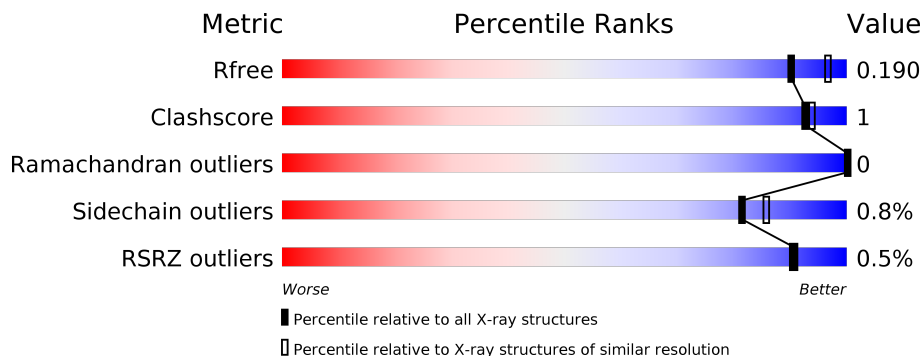
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	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 $\leq 5\%$. 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	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

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.

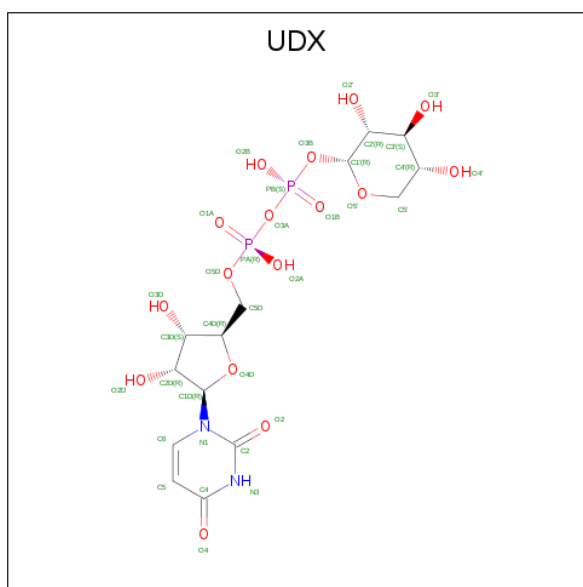
- Molecule 1 is a protein called UDP-glucose 6-dehydrogenase.

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

There are 6 discrepancies between the modelled and reference sequences:

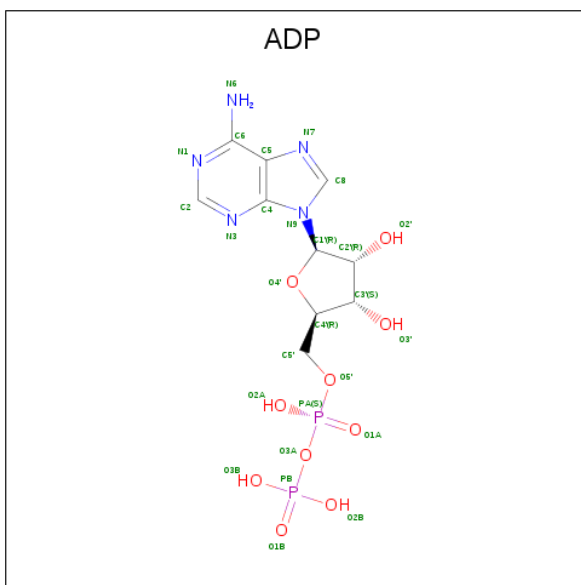
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP O60701
B	0	HIS	-	expression tag	UNP O60701
C	0	HIS	-	expression tag	UNP O60701
D	0	HIS	-	expression tag	UNP O60701
E	0	HIS	-	expression tag	UNP O60701
F	0	HIS	-	expression tag	UNP O60701

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-XYLOPYRANOSE (three-letter code: UDX) (formula: C₁₄H₂₂N₂O₁₆P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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 ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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


- Molecule 4 is water.

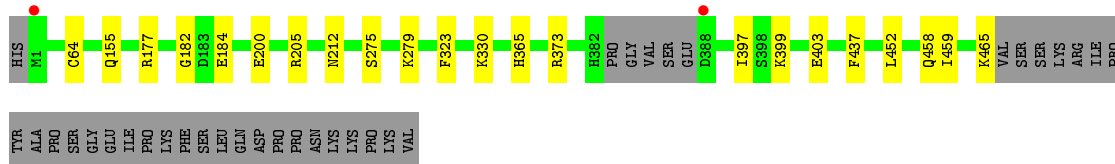
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	233	Total	O	0	0
			233	233		
4	C	188	Total	O	0	0
			188	188		
4	D	209	Total	O	0	0
			209	209		
4	E	138	Total	O	0	0
			138	138		
4	F	126	Total	O	0	0
			126	126		

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.

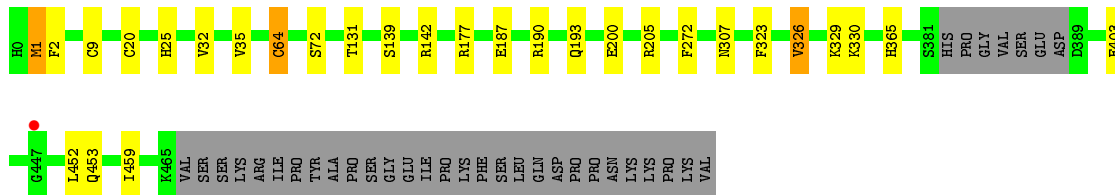
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain A:  88% 7%

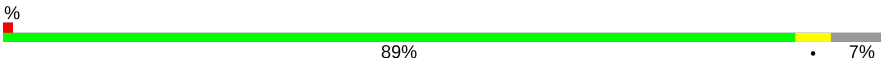


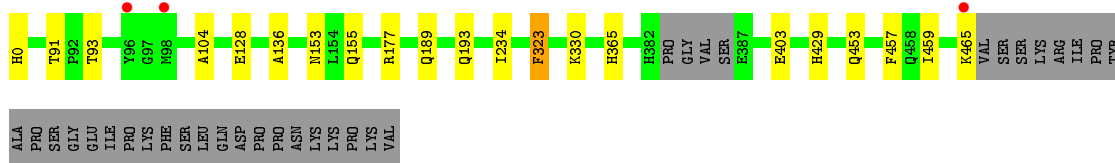
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain B:  87% 5% 7%




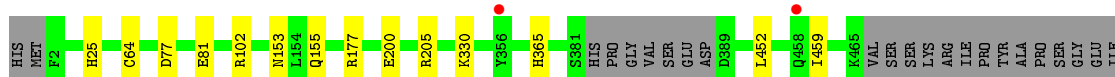
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain C:  89% 7%



- Molecule 1: UDP-glucose 6-dehydrogenase

Chain D:  89% 8%



PRO
LYS
PHE
SER
LEU
GLN
ASP
PRO
PRO
ASN
LYS
LYS
PRO
LYS
VAL

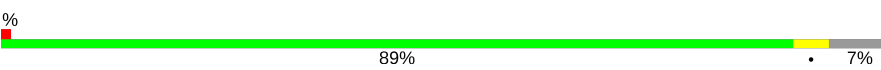
- Molecule 1: UDP-glucose 6-dehydrogenase

Chain E:  91% 8%

HIS MET F2 C64 M453 L194 Q195 R177 K267 F323 K330 H365 S381 HIS PRO GLY VAL SER GLU ASP D389 G447 K465 VAL SER LYS ARG ILE PRO TYR ALA PRO SER GLY ILE PRO LYS PHE SER LEU GLN ASP PRO ASN LYS PRO

LYS
VAL

- Molecule 1: UDP-glucose 6-dehydrogenase

Chain F:  % 89% 7%

HIS MI 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 Q488 I459 K465 VAL SER SER LYS ARG

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

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.00Å)	Xtrriage
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	Xtrriage
Anisotropy	0.434	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtrriage
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

Xtrriage'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.*

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: 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.

All (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
1:B:1:MET:HG2	1:B:2:PHE:N	2.16	0.60
1:E:330:LYS:HE3	1:E:365:HIS:CD2	2.40	0.57
1:F:330:LYS:HE3	1:F:365:HIS:CG	2.40	0.56
1:B:272:PHE:N	1:B:307:ASN:HD21	2.04	0.56
1:C:403:GLU:HG2	4:C:628:HOH:O	2.06	0.55
1:B:330:LYS:HE3	1:B:365:HIS:CG	2.41	0.55
1:A:200:GLU:OE2	1:A:205:ARG:HD3	2.07	0.54
1:F:91:THR:HG21	1:F:104:ALA:HB1	1.90	0.53
1:C:91:THR:HG21	1:C:104:ALA:HB1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:GLU:HG2	4:B:605:HOH:O	2.08	0.52
1:B:453:GLN:HG3	1:B:459:ILE:HD12	1.92	0.51
1:C:330:LYS:HE3	1:C:365:HIS:CG	2.46	0.51
1:D:330:LYS:HE3	1:D:365:HIS:CG	2.46	0.51
1:C:91:THR:CG2	1:C:104:ALA:HB1	2.41	0.50
1:D:200:GLU:OE2	1:D:205:ARG:HD3	2.12	0.50
1:E:330:LYS:HE3	1:E:365:HIS:CG	2.47	0.50
1:A:155:GLN:NE2	4:A:602:HOH:O	2.40	0.49
1:D:452:LEU:HB2	1:D:459:ILE:HD11	1.95	0.49
1:A:184:GLU:HG2	4:A:620:HOH:O	2.13	0.49
1:F:37:VAL:HG13	3:F:500:ADP:C2	2.49	0.47
1:F:446:ASP:O	4:F:601:HOH:O	2.19	0.47
1:B:326:VAL:HA	1:B:329:LYS:HD2	1.96	0.47
1:D:153:ASN:OD1	1:D:155:GLN:NE2	2.48	0.46
1:A:330:LYS:HE3	1:A:365:HIS:CG	2.50	0.46
1:A:403:GLU:HG2	4:A:618:HOH:O	2.15	0.46
1:D:102:ARG:HD2	4:D:673:HOH:O	2.15	0.46
1:B:330:LYS:HE3	1:B:365:HIS:CD2	2.51	0.46
1:A:437:PHE:CE2	1:A:458:GLN:HG2	2.50	0.45
1:B:326:VAL:HG23	1:B:326:VAL:O	2.15	0.45
1:F:91:THR:HG22	1:F:104:ALA:HB1	1.99	0.45
1:A:399:LYS:HA	1:A:399:LYS:HD3	1.78	0.45
1:B:200:GLU:OE2	1:B:205:ARG:HD3	2.16	0.45
1:B:9:CYS:HB2	1:B:20:CYS:SG	2.57	0.44
1:D:330:LYS:HE3	1:D:365:HIS:CD2	2.52	0.44
1:F:437:PHE:CE2	1:F:458:GLN:HG2	2.52	0.44
1:C:189:GLN:O	1:C:193:GLN:HG2	2.16	0.44
1:C:453:GLN:HG3	1:C:459:ILE:HD13	2.00	0.43
1:C:153:ASN:OD1	1:C:155:GLN:NE2	2.51	0.43
1:B:142:ARG:HD3	1:C:323:PHE:CE1	2.54	0.43
1:F:373:ARG:HG3	1:F:397:ILE:HG21	1.99	0.43
1:F:330:LYS:HE3	1:F:365:HIS:CD2	2.54	0.43
1:C:155:GLN:OE1	4:C:601:HOH:O	2.21	0.43
1:B:20:CYS:HB3	1:B:32:VAL:HG11	2.02	0.42
1:B:131:THR:OG1	2:B:501:UDX:H2'1	2.20	0.42
1:F:93:THR:HG21	1:F:101:GLY:C	2.39	0.41
1:C:128:GLU:HG3	1:C:136:ALA:HB1	2.02	0.41
1:A:452:LEU:CB	1:A:459:ILE:HD11	2.51	0.41
1:B:25:HIS:HA	1:B:64:CYS:SG	2.60	0.41
1:C:429:HIS:HB2	1:C:457:PHE:CZ	2.56	0.41
1:A:373:ARG:HG3	1:A:397:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:LYS:HE3	1:C:365:HIS:CD2	2.56	0.41
1:A:182:GLY:O	1:A:212:ASN:HA	2.20	0.41
1:A:275:SER:O	1:A:279:LYS:NZ	2.54	0.40
1:B:35:VAL:HA	1:B:72:SER:O	2.21	0.40
1:B:139:SER:HB3	1:C:323:PHE:CE2	2.57	0.40
1:D:25:HIS:HE1	4:D:788:HOH:O	2.04	0.40
1:B:330:LYS:HE3	1:B:365:HIS:CE1	2.56	0.40
1:D:77:ASP:O	1:D:81:GLU:HG2	2.22	0.40
1:C:234:ILE:HA	1:C:234:ILE:HD12	1.97	0.40
1:F:128:GLU:HG3	1:F:136:ALA:HB1	2.03	0.40

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

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ARG
1	A	323	PHE
1	A	465	LYS
1	B	1	MET
1	B	177	ARG
1	B	193	GLN
1	B	323	PHE
1	B	326	VAL
1	C	0	HIS
1	C	93	THR
1	C	177	ARG
1	C	323	PHE
1	C	465	LYS
1	D	177	ARG
1	E	177	ARG
1	E	267	LYS
1	F	177	ARG
1	F	193	GLN
1	F	323	PHE
1	F	459	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	B	193	GLN
1	B	307	ASN
1	C	155	GLN
1	C	201	HIS
1	C	301	GLN
1	D	118	GLN
1	D	159	ASN
1	D	363	HIS
1	E	365	HIS
1	F	25	HIS
1	F	155	GLN
1	F	159	ASN
1	F	229	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

All (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
2	E	502	UDX	O4D-C1D	2.24	1.44	1.41
2	B	502	UDX	O4D-C1D	2.16	1.44	1.41
2	A	501	UDX	C2-N3	-2.15	1.33	1.38
2	C	501	UDX	O4D-C1D	2.10	1.44	1.41
2	E	501	UDX	O4D-C1D	2.08	1.44	1.41
2	B	501	UDX	C2-N3	-2.07	1.34	1.38
2	E	501	UDX	C2-N3	-2.06	1.34	1.38
2	D	502	UDX	C2-N3	-2.04	1.34	1.38
2	E	502	UDX	C2-N3	-2.01	1.34	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	B	501	UDX	O3B-C1'-C2'	2.92	113.73	108.38
3	C	500	ADP	C4-C5-N7	-2.88	106.39	109.40
2	D	502	UDX	O5'-C1'-O3B	-2.87	107.61	111.36
2	A	501	UDX	O3B-C1'-C2'	2.86	113.62	108.38
2	C	501	UDX	O5'-C1'-O3B	-2.79	107.71	111.36
3	C	500	ADP	C1'-N9-C4	-2.77	121.78	126.64
2	B	502	UDX	O5'-C5'-C4'	-2.71	106.59	110.77
2	E	501	UDX	O3B-C1'-C2'	2.59	113.13	108.38
2	D	501	UDX	O4D-C1D-C2D	-2.49	103.29	106.93
2	B	502	UDX	O4D-C1D-C2D	-2.36	103.47	106.93
2	B	501	UDX	C1'-C2'-C3'	2.31	114.81	110.00
2	A	502	UDX	O4D-C1D-C2D	-2.30	103.57	106.93
2	E	502	UDX	O4D-C1D-C2D	-2.28	103.60	106.93
2	A	502	UDX	O3A-PB-O3B	2.27	107.07	102.48
2	C	501	UDX	O2'-C2'-C1'	-2.10	104.94	110.05
2	E	501	UDX	C5'-C4'-C3'	2.10	112.24	109.67
2	F	501	UDX	O5'-C5'-C4'	-2.07	107.57	110.77
2	A	501	UDX	O5'-C5'-C4'	-2.05	107.61	110.77

There are no chirality outliers.

All (38) torsion outliers are listed below:

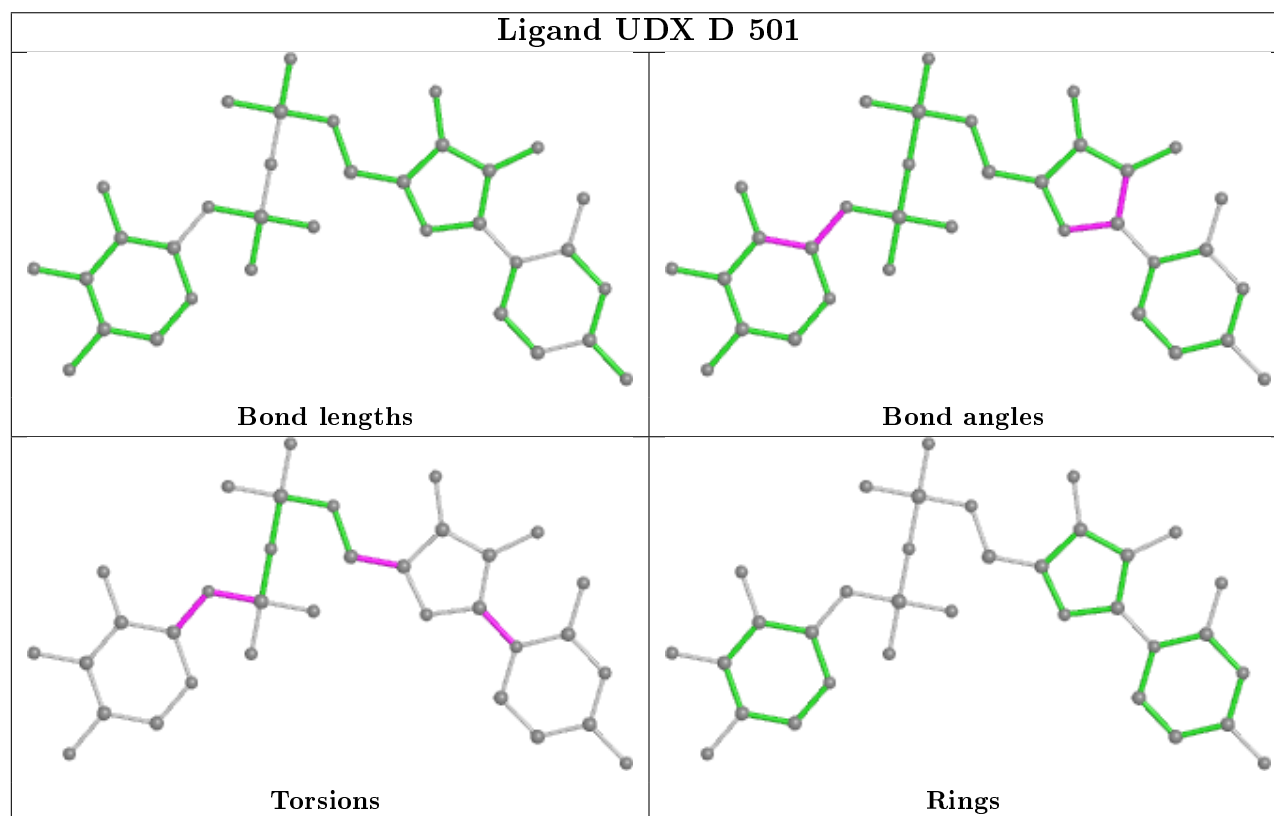
Mol	Chain	Res	Type	Atoms
2	D	501	UDX	C1'-O3B-PB-O2B
2	D	501	UDX	O4D-C1D-N1-C6
2	D	501	UDX	C2D-C1D-N1-C6
2	A	501	UDX	C1'-O3B-PB-O2B
2	A	501	UDX	O4D-C1D-N1-C6
2	A	501	UDX	C2D-C1D-N1-C6
2	B	501	UDX	C1'-O3B-PB-O2B
2	B	501	UDX	O4D-C1D-N1-C6
2	B	501	UDX	C2D-C1D-N1-C6
2	B	502	UDX	PA-O3A-PB-O3B
2	E	501	UDX	C1'-O3B-PB-O2B
2	E	501	UDX	O4D-C1D-N1-C6
2	E	501	UDX	C2D-C1D-N1-C6
2	D	501	UDX	C1'-O3B-PB-O3A
2	A	501	UDX	C1'-O3B-PB-O3A
2	B	501	UDX	C1'-O3B-PB-O3A
2	D	502	UDX	C1'-O3B-PB-O3A
2	E	502	UDX	C1'-O3B-PB-O3A
2	C	501	UDX	C1'-O3B-PB-O3A
2	A	502	UDX	C1'-O3B-PB-O3A
2	E	501	UDX	C1'-O3B-PB-O3A
2	F	501	UDX	C1'-O3B-PB-O3A
2	B	502	UDX	C1'-O3B-PB-O3A
2	D	502	UDX	PA-O3A-PB-O3B
2	C	501	UDX	PA-O3A-PB-O3B
2	A	502	UDX	PA-O3A-PB-O3B
2	B	501	UDX	C2'-C1'-O3B-PB
2	B	502	UDX	PB-O3A-PA-O1A
3	C	500	ADP	O4'-C4'-C5'-O5'
3	F	500	ADP	O4'-C4'-C5'-O5'
2	C	501	UDX	PB-O3A-PA-O1A
2	A	502	UDX	PB-O3A-PA-O1A
2	D	501	UDX	C2'-C1'-O3B-PB
2	A	501	UDX	C2'-C1'-O3B-PB
2	B	501	UDX	O4D-C4D-C5D-O5D
2	D	501	UDX	O4D-C4D-C5D-O5D
2	A	501	UDX	O4D-C4D-C5D-O5D
2	E	501	UDX	O4D-C4D-C5D-O5D

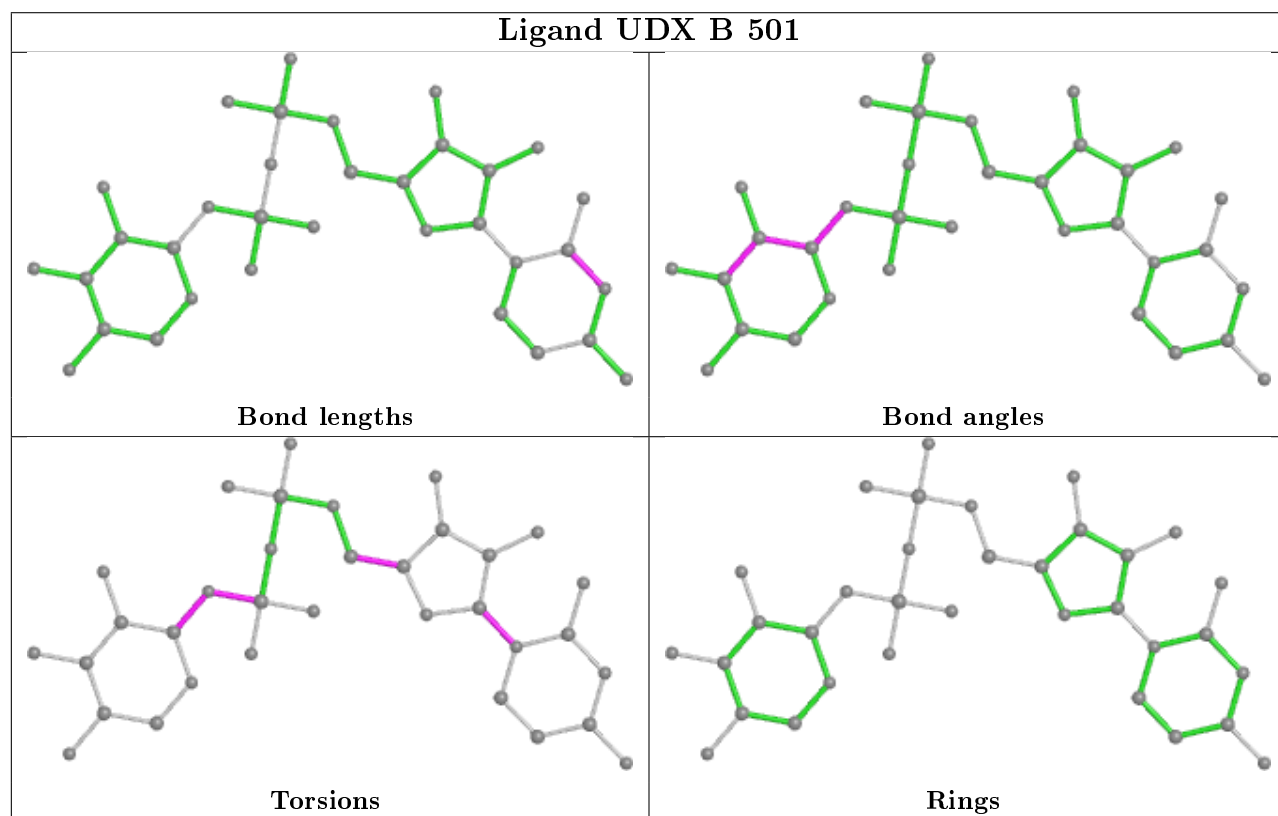
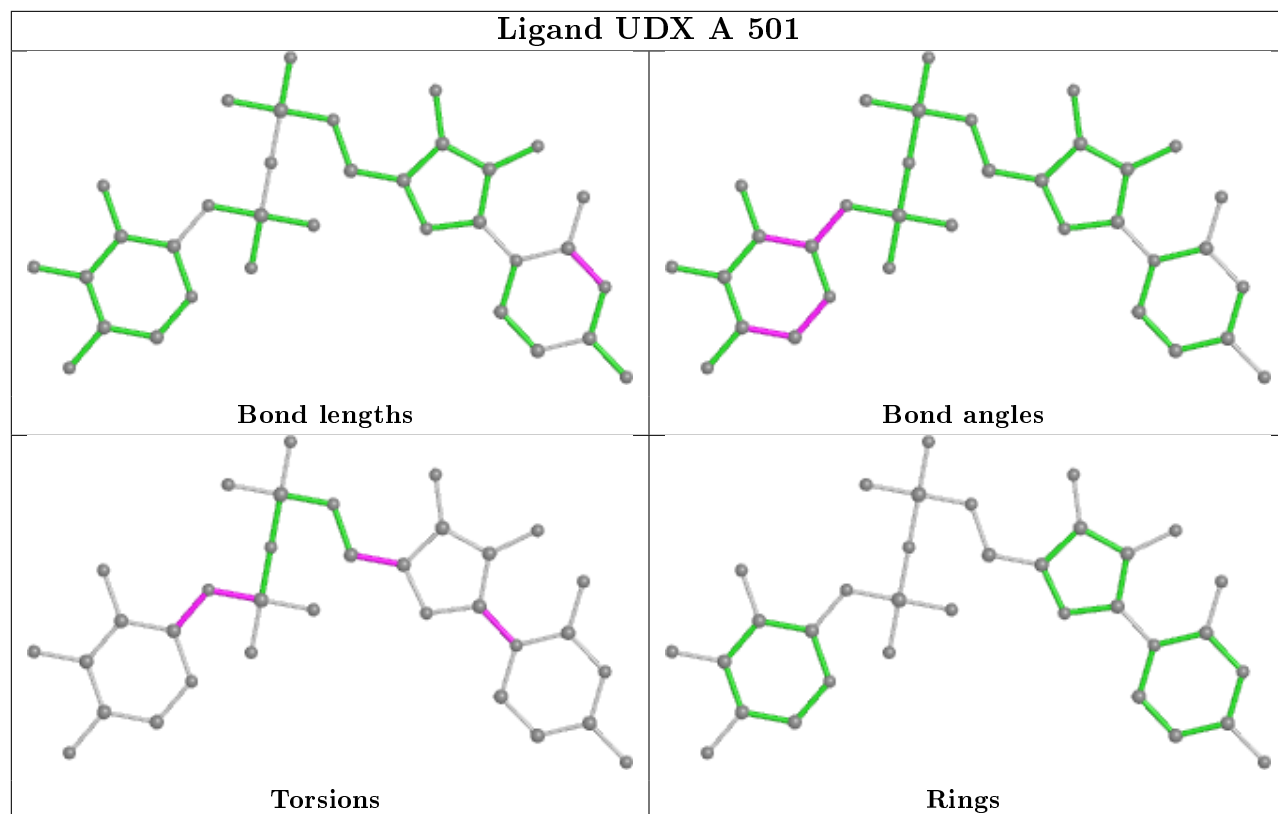
There are no ring outliers.

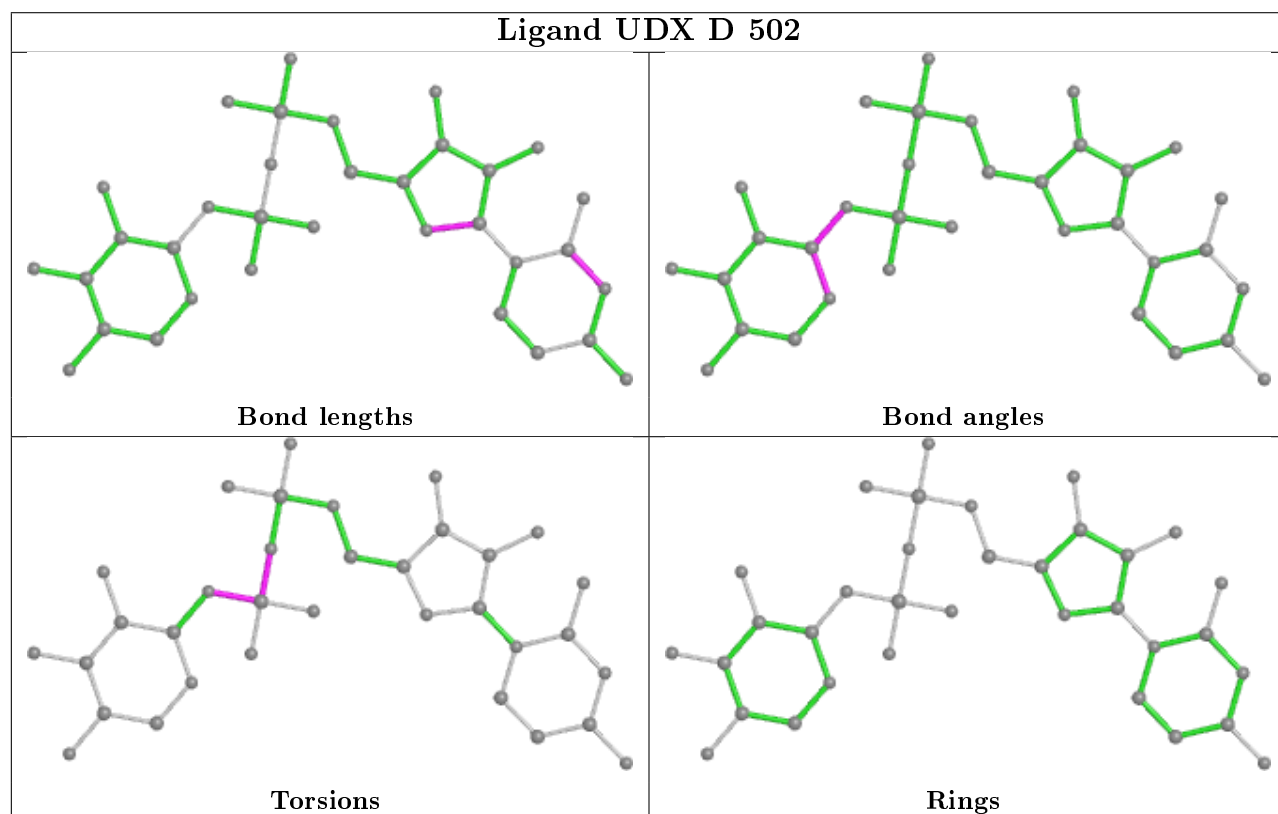
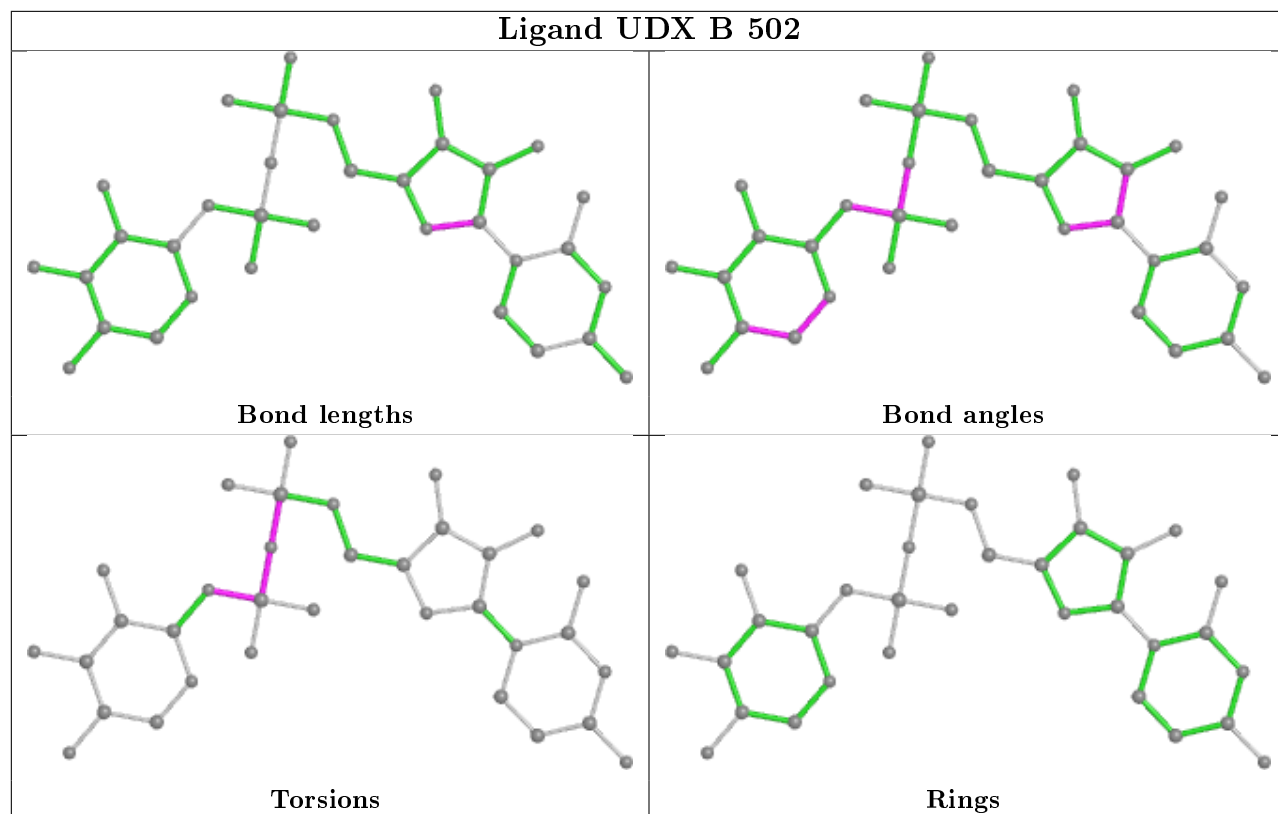
2 monomers are involved in 2 short contacts:

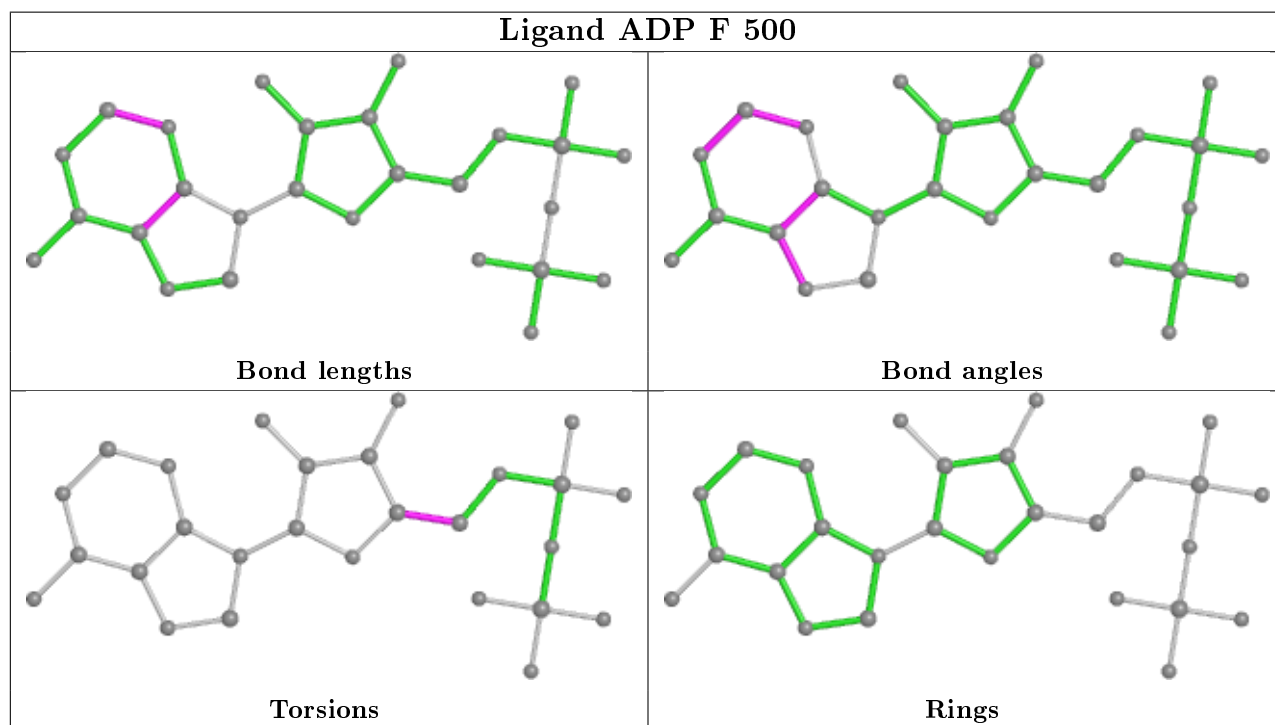
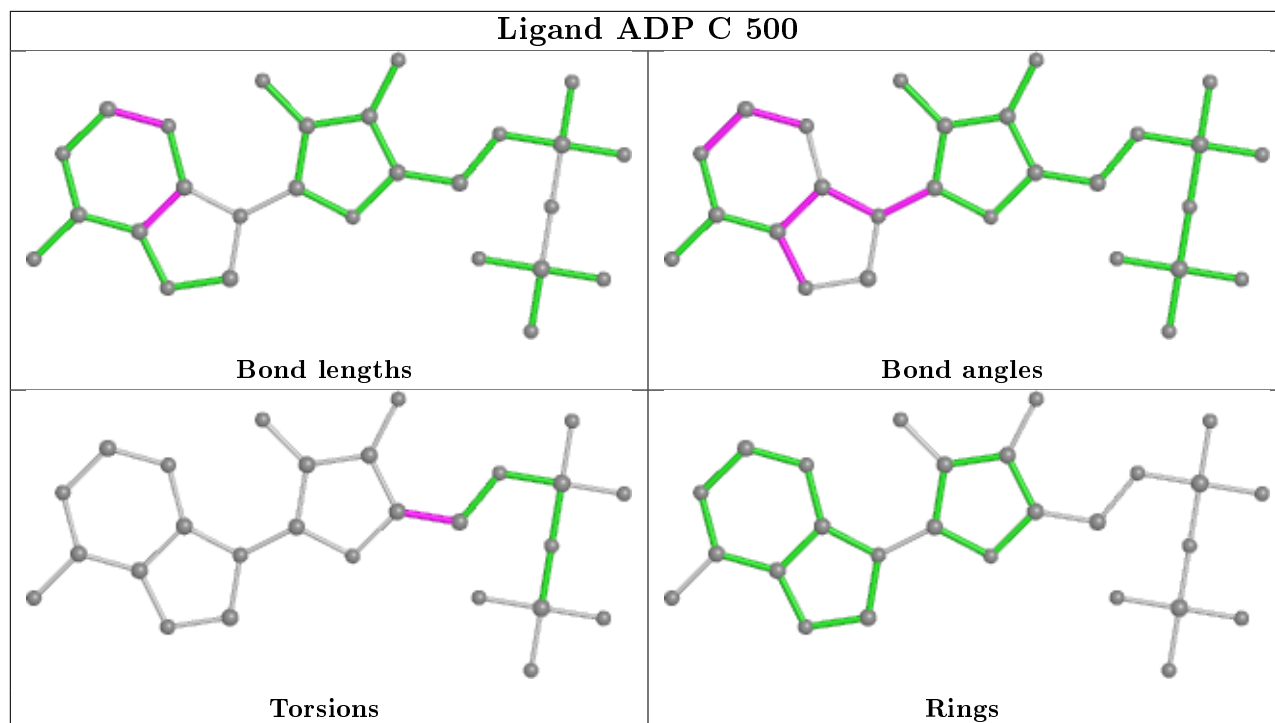
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	UDX	1	0
3	F	500	ADP	1	0

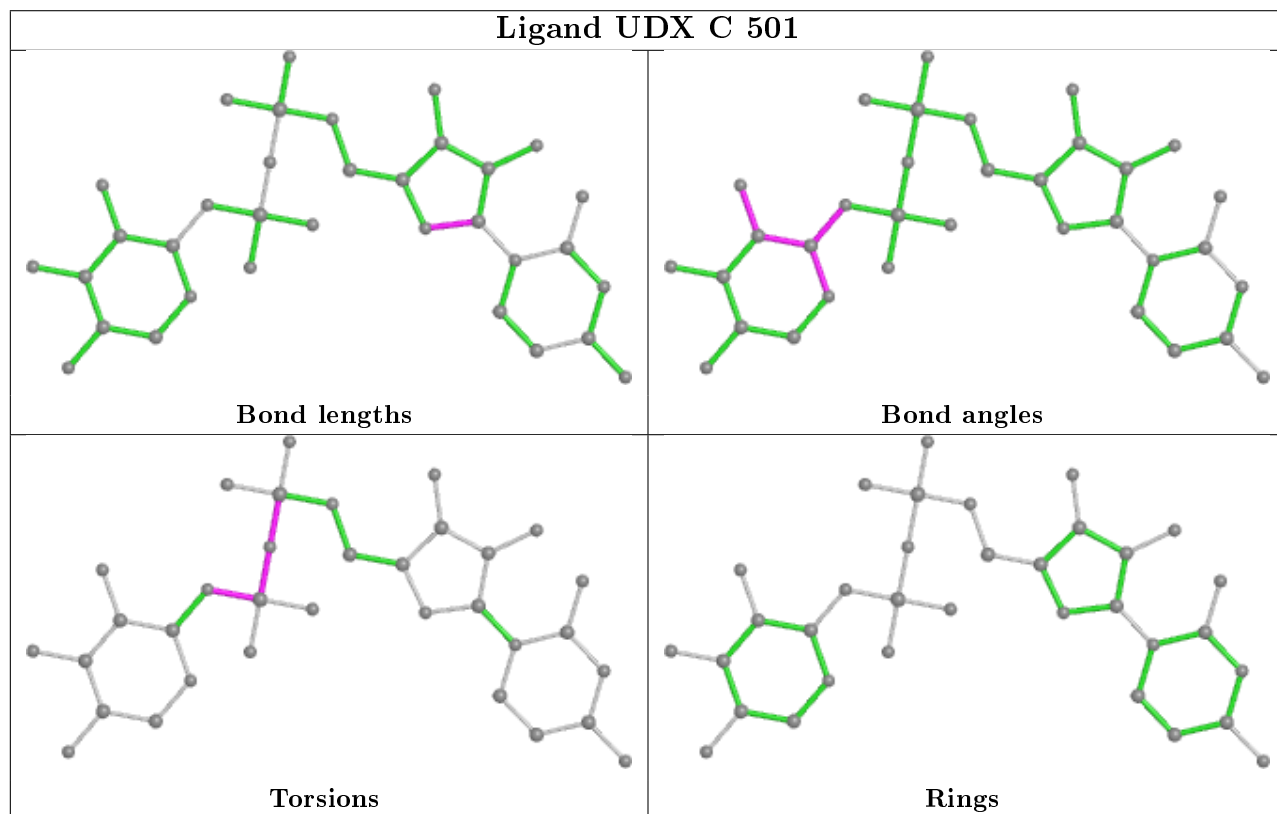
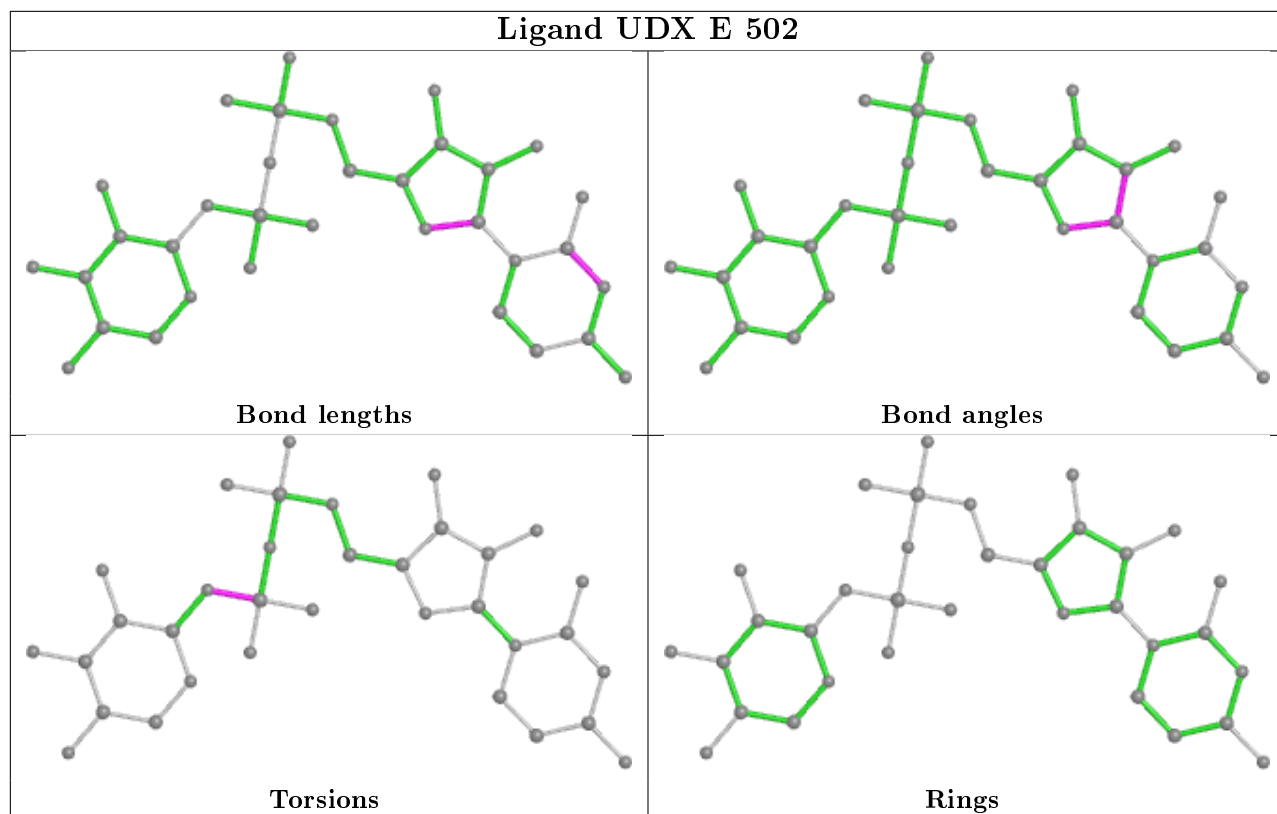
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

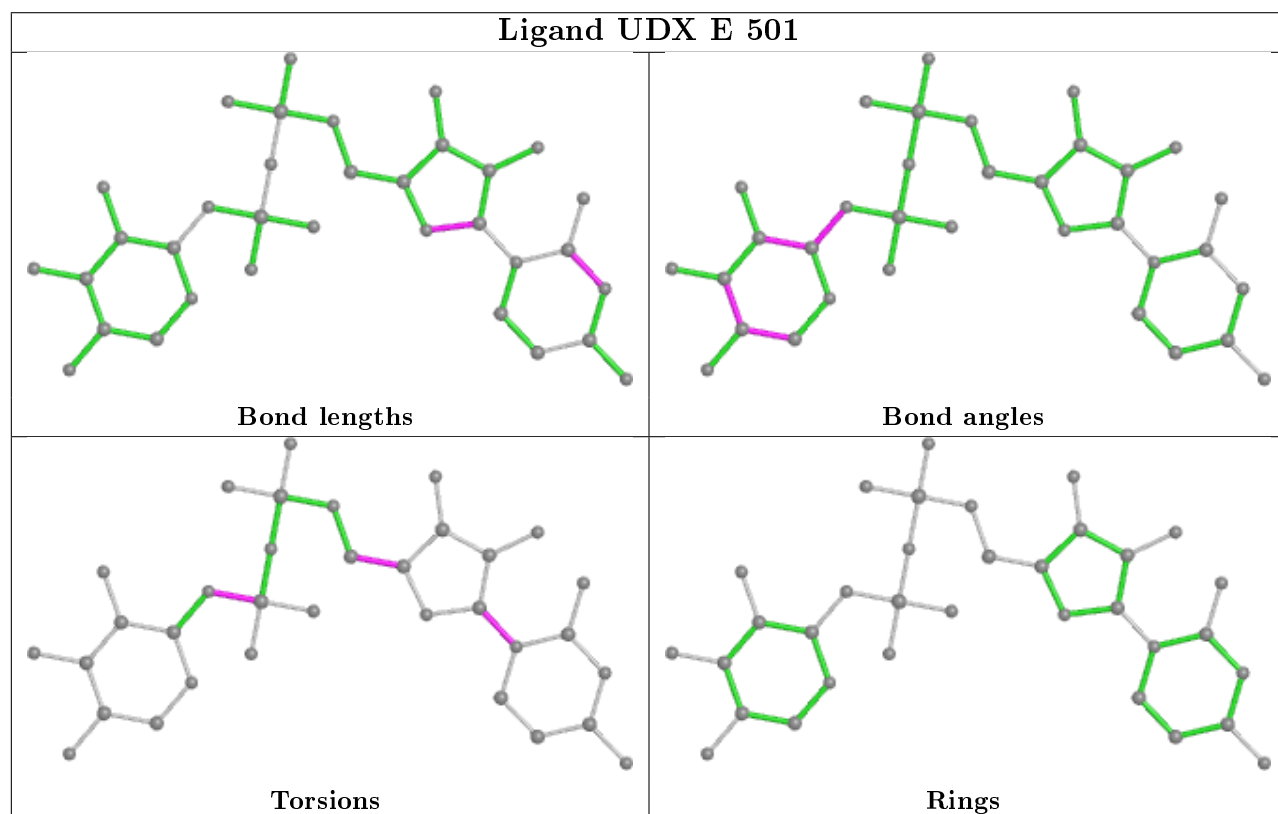
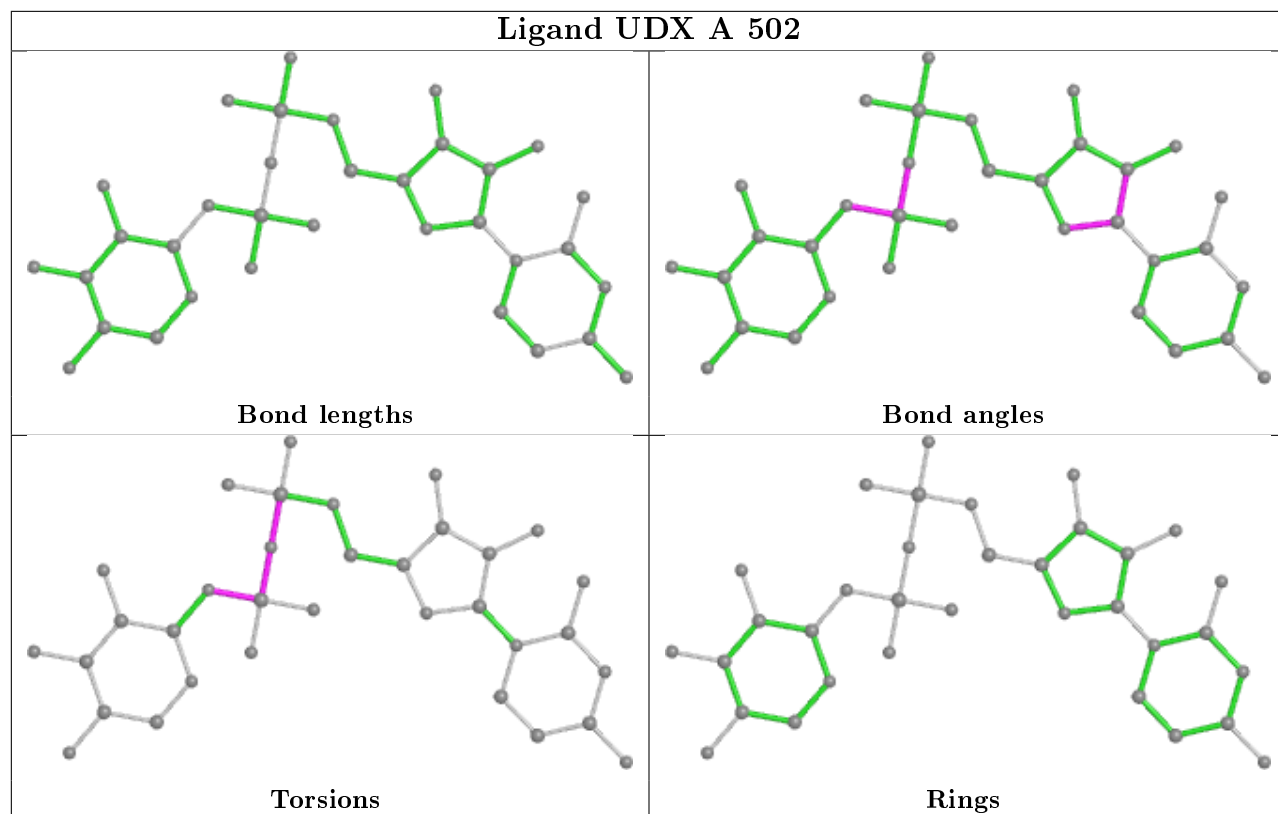


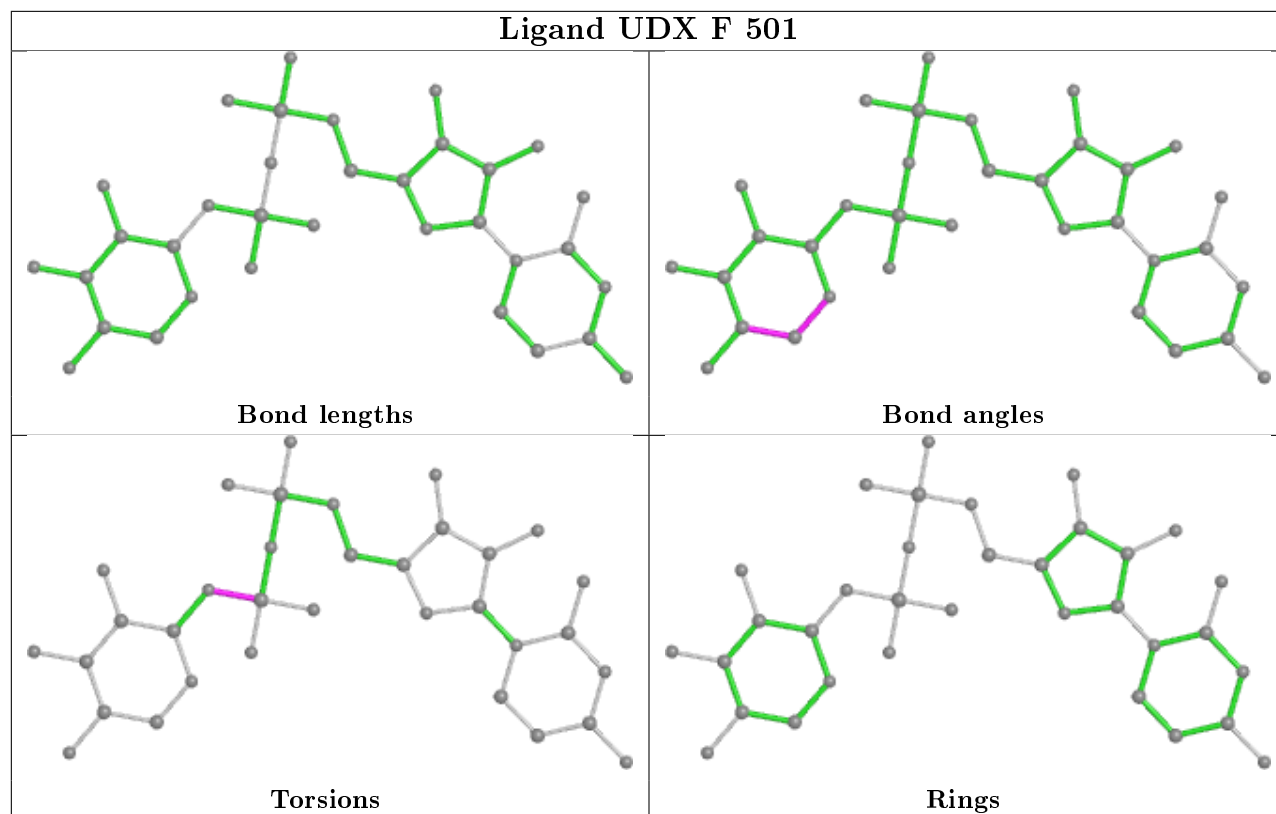












5.7 Other polymers [i](#)

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 [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

All (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
1	F	96	TYR	3.0
1	F	1	MET	2.7
1	A	1	MET	2.6
1	D	458	GLN	2.6
1	C	96	TYR	2.2
1	F	108	TYR	2.2
1	B	447	GLY	2.1
1	E	323	PHE	2.1
1	A	388	ASP	2.1

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](#)

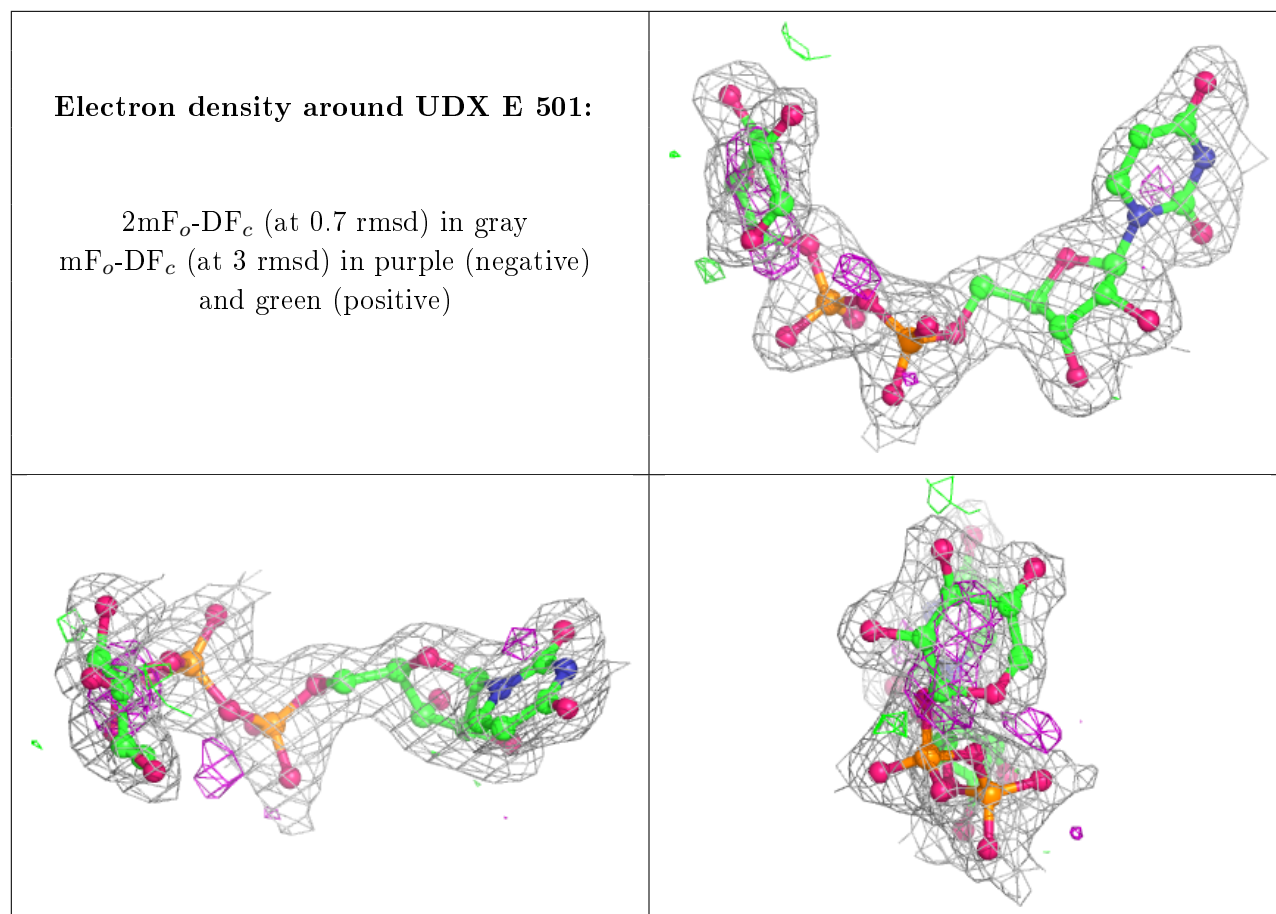
There are no carbohydrates in this entry.

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.

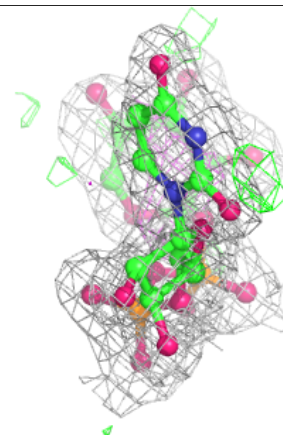
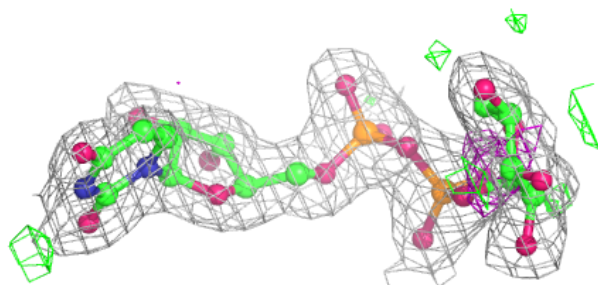
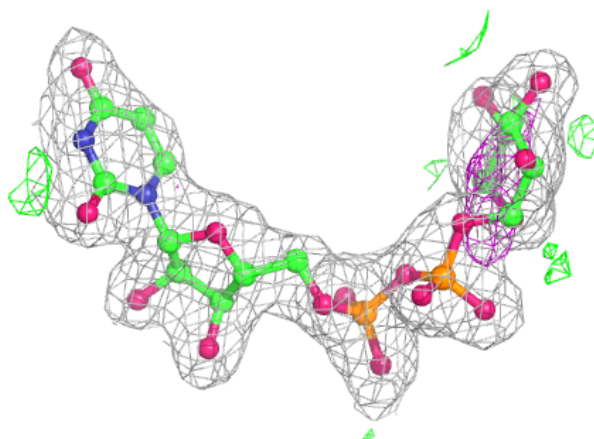
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UDX	E	501	34/34	0.96	0.13	27,36,54,56	0
2	UDX	A	501	34/34	0.97	0.12	22,30,47,48	0
2	UDX	B	501	34/34	0.97	0.13	18,26,44,46	0
3	ADP	F	500	27/27	0.97	0.10	31,39,47,54	0
2	UDX	D	501	34/34	0.97	0.12	19,29,51,52	0
2	UDX	E	502	34/34	0.98	0.10	18,22,25,29	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.



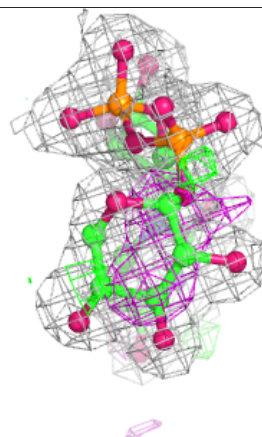
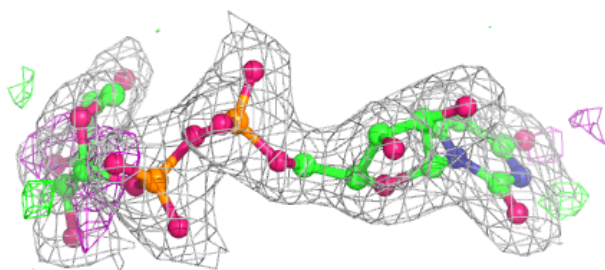
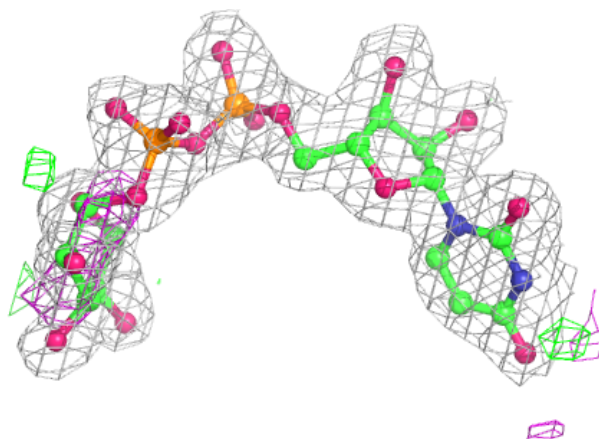
Electron density around UDX A 501:

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

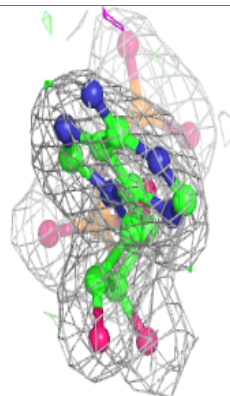
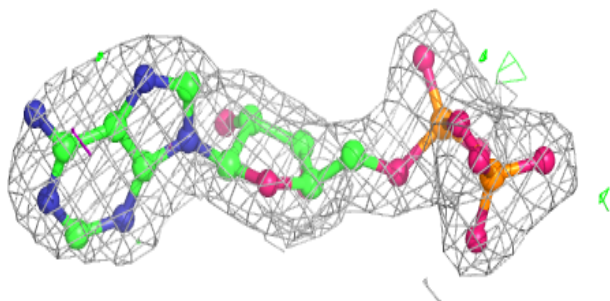
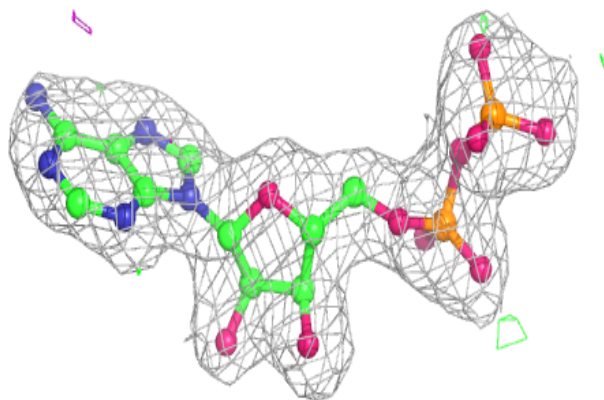


Electron density around UDX B 501:

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

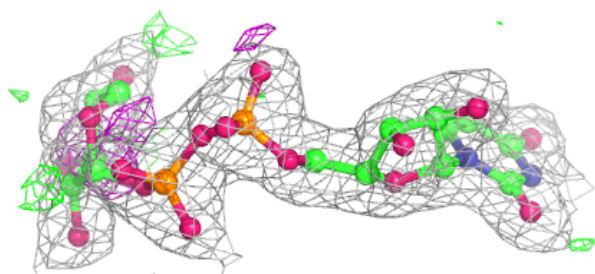
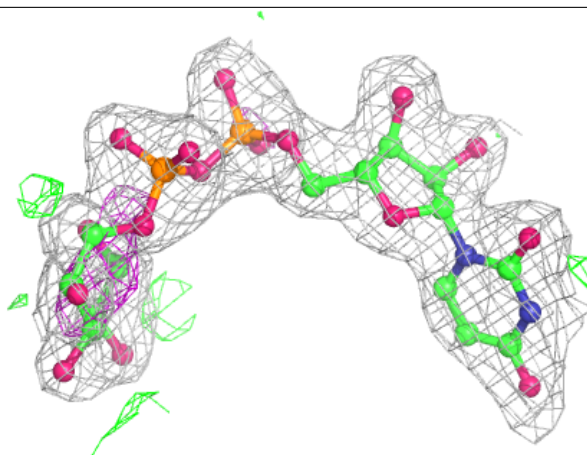
**Electron density around ADP F 500:**

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

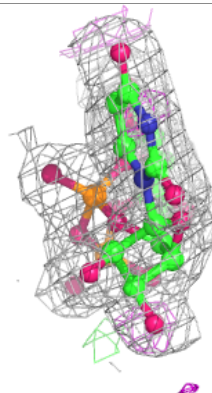
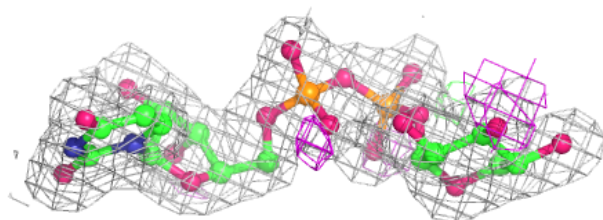
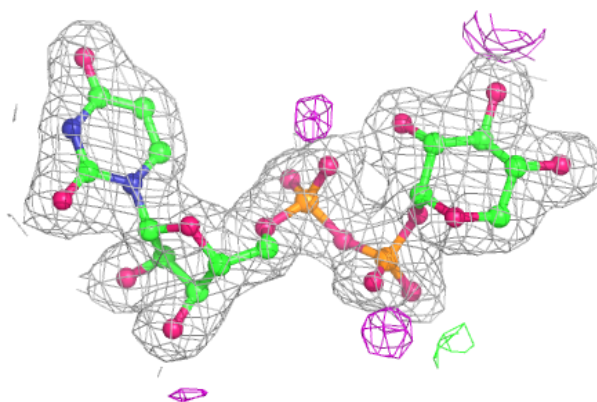


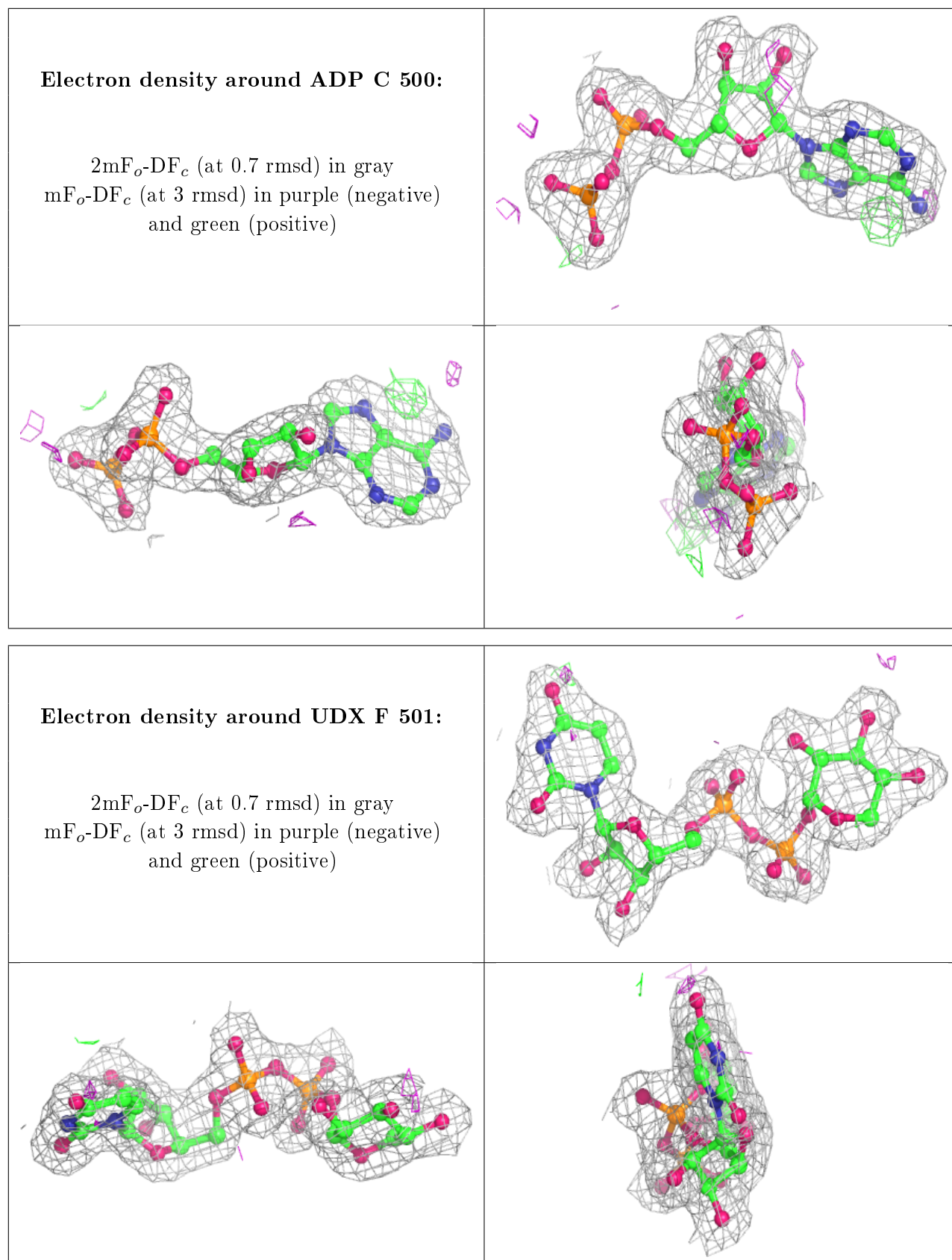
Electron density around UDX D 501:

$2mF_o-DF_c$ (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:**

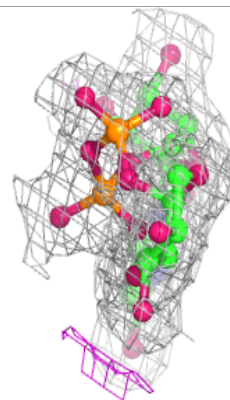
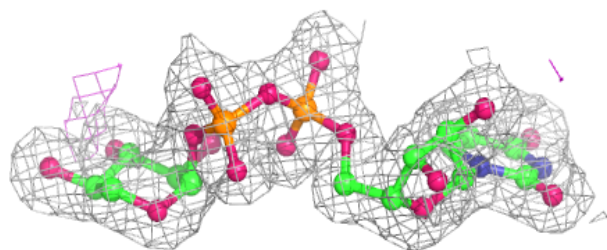
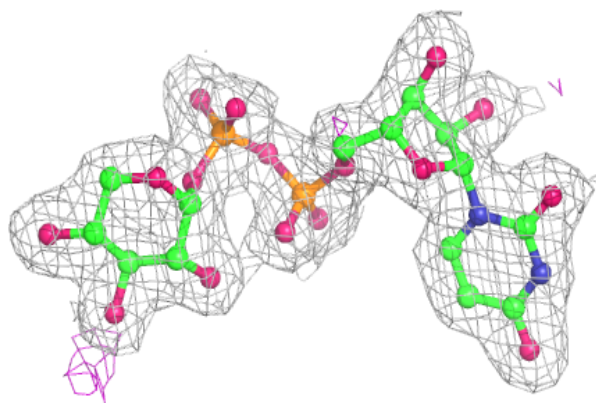
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



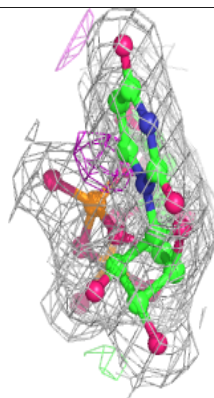
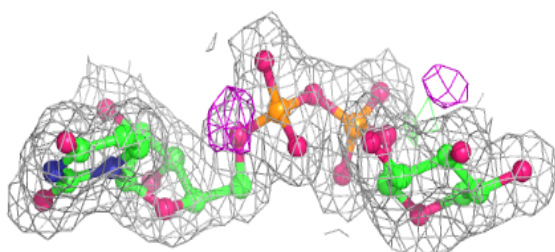
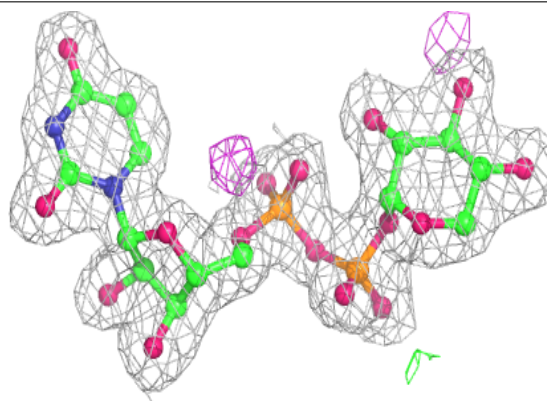


Electron density around UDX C 501:

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

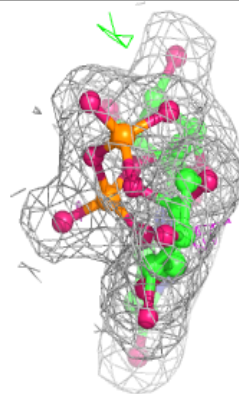
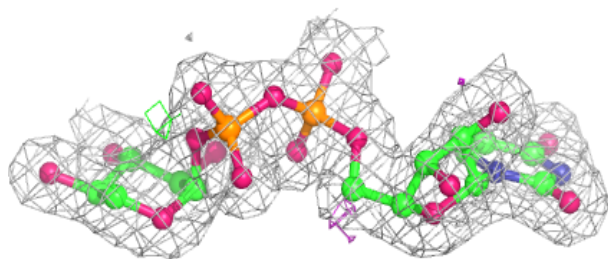
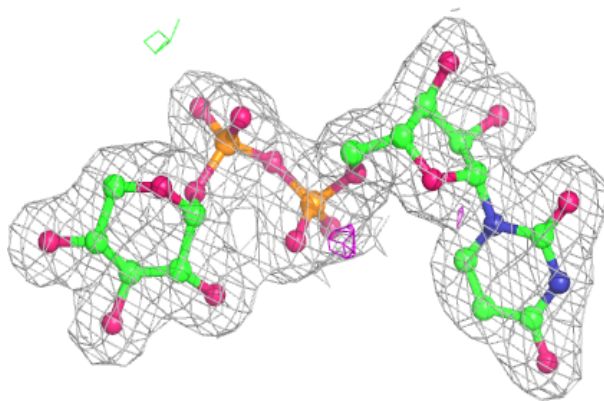
**Electron density around UDX A 502:**

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

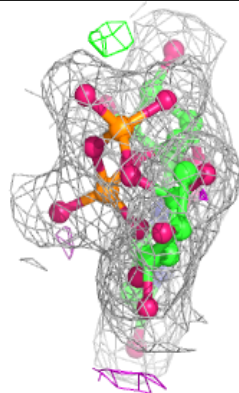
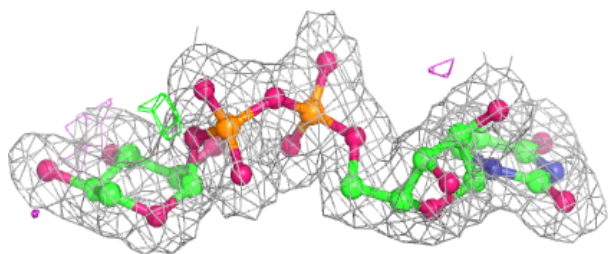
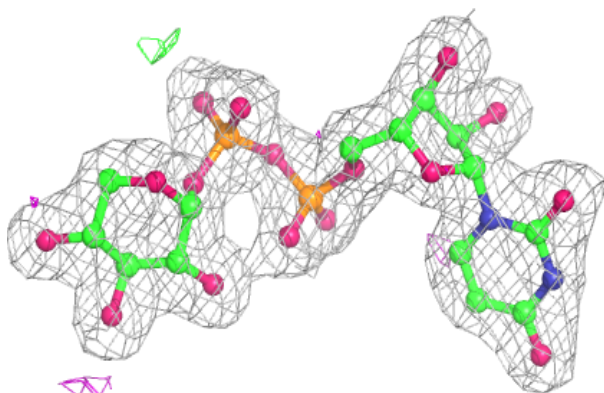


Electron density around UDX D 502:

$2mF_o-DF_c$ (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

There are no such residues in this entry.