



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:59 AM UTC

PDB ID : 5VR8 / pdb_00005vr8
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

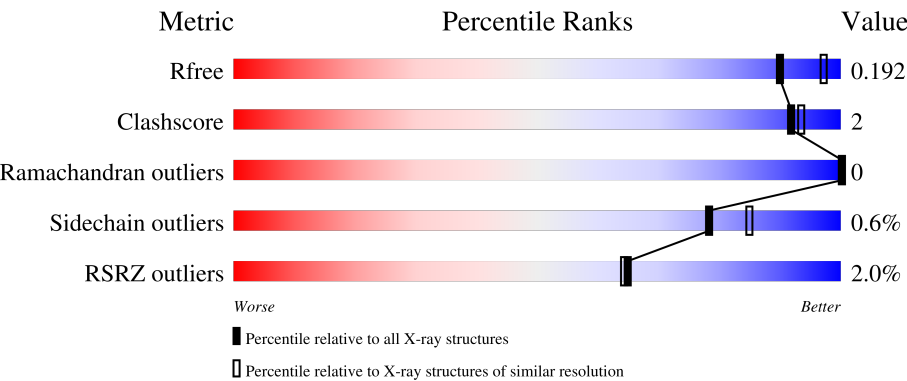
1 Overall quality at a glance i

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	495	89%7%
1	B	495	86%6%7%
1	C	495	89%7%
1	D	495	90%8%
1	E	495	91%8%

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Mol	Chain	Length	Quality of chain
1	F	495	2% 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.

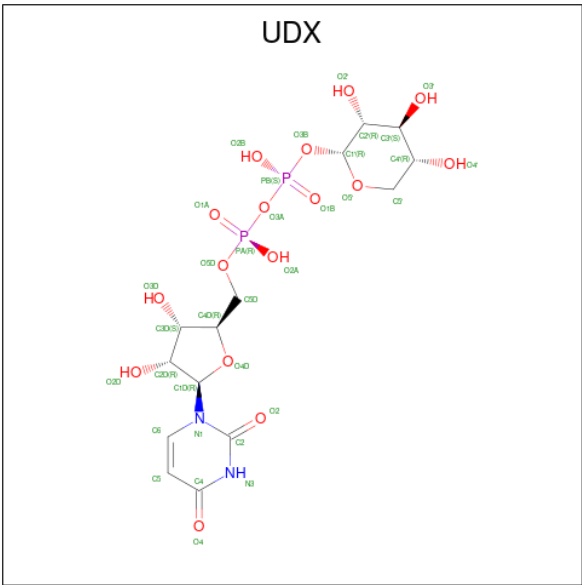
- Molecule 1 is a protein called UDP-glucose 6-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 (CCD ID: 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 ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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		

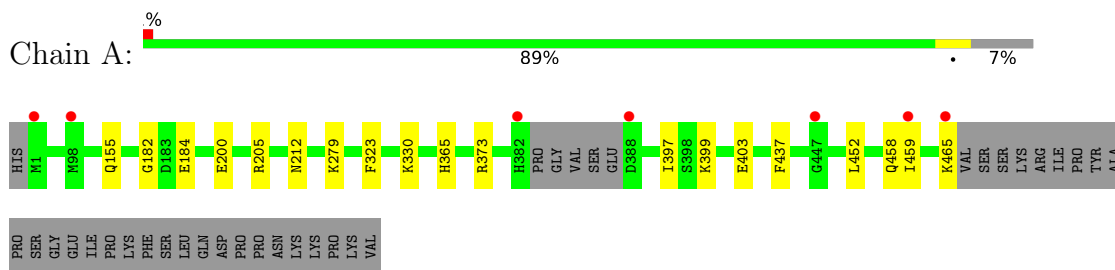
- Molecule 4 is water.

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		

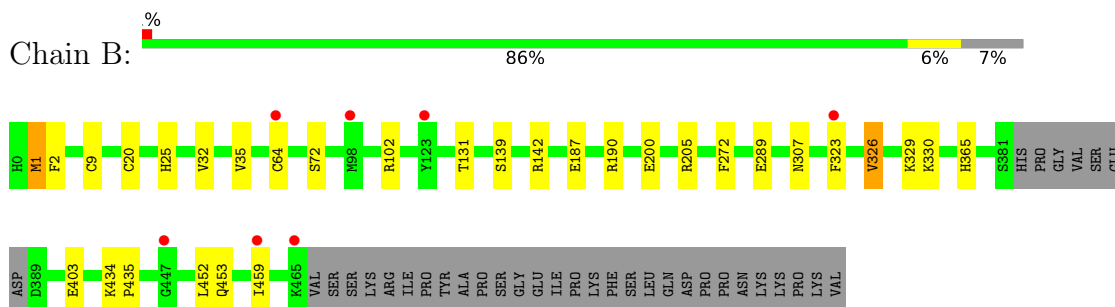
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

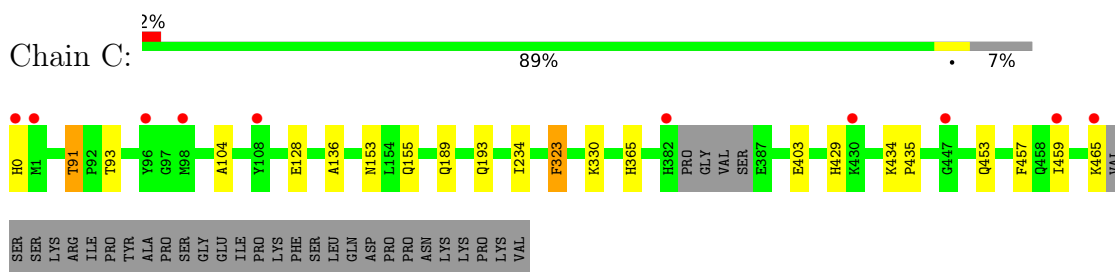
- Molecule 1: UDP-glucose 6-dehydrogenase



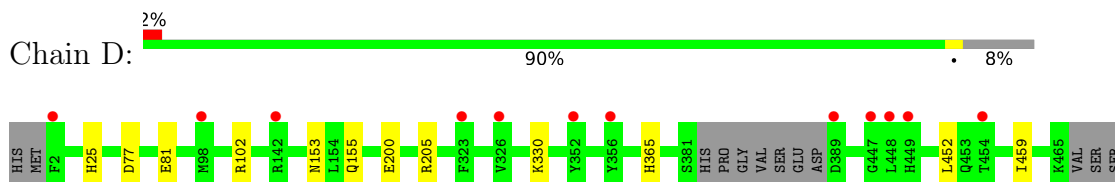
- Molecule 1: UDP-glucose 6-dehydrogenase



- Molecule 1: UDP-glucose 6-dehydrogenase

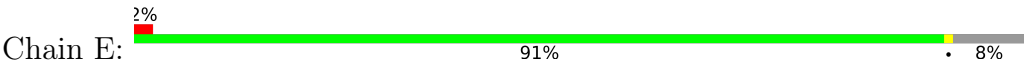


- Molecule 1: UDP-glucose 6-dehydrogenase



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
LYS
VAL

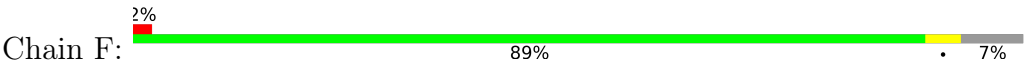
● Molecule 1: UDP-glucose 6-dehydrogenase



HIS
MET
F2
M98
M153
L164
Q155
F323
Y326
K330
H365
S381
HIS
PRO
GLY
VAL
SER
GLU
ASP
D389
K399
D406
G447
L448
H449
T454
K465
VAL
SER
SER
LYS
ARG
ILE
TYR
PRO
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



HIS
M1
V37
T91
P92
T93
Y96
G97
M98
G101
A104
E128
A136
K149
F323
K330
H365
R373
S381
HIS
PRO
GLY
VAL
SER
GLU
ASP
D389
I397
D406
K434
P435
A436
F437
D446
G447
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
LYS
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 49.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.12-2.00) 93.3 (49.12-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.156 , 0.190 0.160 , 0.192	Depositor DCC
R_{free} test set	11196 reflections (4.69%)	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)	0.35 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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

5.1 Standard geometry

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

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	0.35	0/3672	0.51	0/4967
1	B	0.36	0/3664	0.52	0/4956
1	C	0.34	0/3692	0.51	0/4994
1	D	0.32	0/3645	0.47	0/4931
1	E	0.28	0/3645	0.45	0/4931
1	F	0.28	0/3653	0.45	0/4941
All	All	0.32	0/21971	0.49	0/29720

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3607	0	3622	10	0
1	B	3599	0	3618	23	0
1	C	3626	0	3635	15	0
1	D	3581	0	3599	8	0
1	E	3581	0	3599	4	0
1	F	3589	0	3611	13	0
2	A	68	0	40	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	71	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 2.

All (71) 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	0.58
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:330:LYS:NZ	1:E:406:ASP:O	2.46	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:F:93:THR:HG21	1:F:101:GLY:C	2.39	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:O	1:B:326:VAL:HG23	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:434:LYS:HA	1:B:435:PRO:C	2.43	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:102:ARG:HH12	1:B:289:GLU:CD	2.28	0.42
1:F:330:LYS:NZ	1:F:406:ASP:O	2.50	0.42
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:B:1:MET:HE3	1:B:1:MET:HB3	1.49	0.41
1:C:128:GLU:HG3	1:C:136:ALA:HB1	2.02	0.41
1:F:434:LYS:HA	1:F:435:PRO:C	2.45	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:C:434:LYS:HA	1:C:435:PRO:C	2.46	0.41
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:HD12	1:C:234:ILE:HA	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 ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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%)	73	80
1	B	394/427 (92%)	391 (99%)	3 (1%)	73	80
1	C	397/427 (93%)	392 (99%)	5 (1%)	61	68
1	D	392/427 (92%)	392 (100%)	0	100	100
1	E	392/427 (92%)	392 (100%)	0	100	100
1	F	393/427 (92%)	391 (100%)	2 (0%)	81	87
All	All	2363/2562 (92%)	2350 (99%)	13 (1%)	78	85

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	279	LYS
1	A	323	PHE
1	A	465	LYS
1	B	1	MET
1	B	323	PHE
1	B	326	VAL
1	C	0	HIS
1	C	91	THR
1	C	93	THR
1	C	323	PHE
1	C	465	LYS
1	F	323	PHE
1	F	459	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	159	ASN
1	A	302	GLN
1	A	382	HIS

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Mol	Chain	Res	Type
1	B	159	ASN
1	B	193	GLN
1	B	201	HIS
1	B	302	GLN
1	B	307	ASN
1	C	0	HIS
1	C	155	GLN
1	C	159	ASN
1	C	201	HIS
1	C	301	GLN
1	C	390	GLN
1	D	118	GLN
1	D	155	GLN
1	D	278	GLN
1	D	363	HIS
1	D	429	HIS
1	E	119	ASN
1	E	121	ASN
1	E	159	ASN
1	F	25	HIS
1	F	155	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 oligosaccharides 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	A	502	-	35,36,36	1.06	3 (8%)	52,55,55	1.51	6 (11%)
2	UDX	B	501	-	35,36,36	1.14	3 (8%)	52,55,55	1.38	6 (11%)
2	UDX	B	502	-	35,36,36	1.05	1 (2%)	52,55,55	1.42	5 (9%)
2	UDX	F	501	-	35,36,36	1.03	2 (5%)	52,55,55	1.51	6 (11%)
3	ADP	F	500	-	28,29,29	1.49	4 (14%)	43,45,45	1.84	11 (25%)
2	UDX	E	501	-	35,36,36	1.13	4 (11%)	52,55,55	1.38	5 (9%)
2	UDX	A	501	-	35,36,36	1.13	3 (8%)	52,55,55	1.44	6 (11%)
3	ADP	C	500	-	28,29,29	1.46	4 (14%)	43,45,45	1.73	10 (23%)
2	UDX	D	502	-	35,36,36	1.19	5 (14%)	52,55,55	1.47	7 (13%)
2	UDX	C	501	-	35,36,36	1.07	3 (8%)	52,55,55	1.50	7 (13%)
2	UDX	E	502	-	35,36,36	1.13	5 (14%)	52,55,55	1.38	5 (9%)
2	UDX	D	501	-	35,36,36	1.09	3 (8%)	52,55,55	1.42	6 (11%)

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	A	502	-	-	2/21/54/54	0/3/3/3
2	UDX	B	501	-	-	3/21/54/54	0/3/3/3
2	UDX	B	502	-	-	2/21/54/54	0/3/3/3
2	UDX	F	501	-	-	0/21/54/54	0/3/3/3
3	ADP	F	500	-	-	1/16/32/32	0/3/3/3
2	UDX	E	501	-	-	4/21/54/54	0/3/3/3
2	UDX	A	501	-	-	3/21/54/54	0/3/3/3
3	ADP	C	500	-	-	1/16/32/32	0/3/3/3
2	UDX	D	502	-	-	1/21/54/54	0/3/3/3
2	UDX	C	501	-	-	2/21/54/54	0/3/3/3
2	UDX	E	502	-	-	0/21/54/54	0/3/3/3
2	UDX	D	501	-	-	3/21/54/54	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	500	ADP	C5-C4	4.82	1.47	1.39
3	C	500	ADP	C5-C4	4.79	1.47	1.39
2	D	502	UDX	PA-O3A	3.24	1.63	1.59
2	B	501	UDX	C4-N3	-3.14	1.33	1.38
2	B	502	UDX	C4-N3	-3.06	1.33	1.38
2	E	502	UDX	PA-O3A	3.03	1.62	1.59
2	A	502	UDX	PA-O3A	3.02	1.62	1.59
3	C	500	ADP	C5-C6	2.96	1.49	1.41
3	F	500	ADP	C5-C6	2.95	1.49	1.41
2	A	501	UDX	C4-N3	-2.83	1.33	1.38
3	C	500	ADP	C8-N7	2.81	1.37	1.31
3	F	500	ADP	C8-N7	2.80	1.37	1.31
2	D	501	UDX	C4-N3	-2.74	1.33	1.38
2	A	501	UDX	PA-O3A	2.63	1.62	1.59
2	E	501	UDX	C4-N3	-2.60	1.34	1.38
3	F	500	ADP	PA-O3A	2.47	1.62	1.59
2	C	501	UDX	C4-N3	-2.41	1.34	1.38
2	C	501	UDX	C2-N1	2.40	1.42	1.38
2	A	501	UDX	C2-N3	-2.33	1.33	1.38
2	D	502	UDX	C2-N1	2.32	1.42	1.38
2	C	501	UDX	PB-O3A	2.27	1.62	1.59
2	B	501	UDX	C2-N3	-2.24	1.34	1.38
2	A	502	UDX	PB-O3A	2.24	1.61	1.59
2	E	501	UDX	C2-N3	-2.22	1.34	1.38
2	D	502	UDX	C2-N3	-2.21	1.34	1.38
2	E	502	UDX	PB-O3A	2.18	1.61	1.59
2	E	502	UDX	C2-N3	-2.17	1.34	1.38
2	F	501	UDX	C4-N3	-2.15	1.34	1.38
2	D	501	UDX	C5-C4	-2.15	1.39	1.43
2	E	502	UDX	C4-N3	-2.12	1.35	1.38
2	D	502	UDX	C4-N3	-2.11	1.35	1.38
2	F	501	UDX	PA-O3A	2.09	1.61	1.59
2	D	501	UDX	C2-N3	-2.08	1.34	1.38
2	D	502	UDX	PB-O3A	2.06	1.61	1.59
3	C	500	ADP	C4-N9	-2.04	1.33	1.37
2	E	501	UDX	C5-C4	-2.04	1.39	1.43
2	A	502	UDX	C2-N1	2.03	1.41	1.38
2	E	501	UDX	C2-N1	2.02	1.41	1.38
2	B	501	UDX	C2-N1	2.01	1.41	1.38
2	E	502	UDX	C6-C5	2.01	1.39	1.35

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	UDX	C4-N3-C2	-5.71	119.52	126.61
2	F	501	UDX	C4-N3-C2	-5.54	119.74	126.61
3	F	500	ADP	C5-C4-N3	-5.50	119.14	126.72
2	C	501	UDX	C4-N3-C2	-5.05	120.34	126.61
2	B	502	UDX	C4-N3-C2	-4.81	120.65	126.61
2	D	502	UDX	C4-N3-C2	-4.76	120.70	126.61
2	C	501	UDX	N3-C2-N1	4.67	120.97	114.89
3	C	500	ADP	C5-C4-N3	-4.66	120.30	126.72
2	E	502	UDX	C4-N3-C2	-4.62	120.87	126.61
2	A	502	UDX	C5-C4-N3	4.58	121.22	114.80
2	E	501	UDX	C4-N3-C2	-4.58	120.93	126.61
2	A	501	UDX	C4-N3-C2	-4.58	120.93	126.61
2	F	501	UDX	C5-C4-N3	4.57	121.21	114.80
2	B	502	UDX	C5-C4-N3	4.32	120.84	114.80
2	F	501	UDX	N3-C2-N1	4.23	120.39	114.89
2	E	502	UDX	N3-C2-N1	4.22	120.39	114.89
2	A	501	UDX	N3-C2-N1	4.22	120.39	114.89
2	D	501	UDX	C4-N3-C2	-4.22	121.38	126.61
2	B	501	UDX	C4-N3-C2	-4.19	121.41	126.61
2	E	501	UDX	N3-C2-N1	4.19	120.34	114.89
2	A	502	UDX	N3-C2-N1	4.18	120.33	114.89
3	F	500	ADP	N3-C4-N9	4.14	134.21	127.17
2	B	502	UDX	N3-C2-N1	4.03	120.13	114.89
2	D	501	UDX	O3B-C1'-C2'	3.90	115.53	108.38
2	D	501	UDX	N3-C2-N1	3.81	119.86	114.89
2	D	502	UDX	N3-C2-N1	3.81	119.85	114.89
3	F	500	ADP	C4-C5-N7	-3.81	106.23	110.58
2	D	502	UDX	C5-C4-N3	3.80	120.12	114.80
2	D	502	UDX	O4-C4-C5	-3.73	118.73	125.16
2	B	501	UDX	C5-C4-N3	3.73	120.02	114.80
2	B	501	UDX	N3-C2-N1	3.72	119.73	114.89
3	C	500	ADP	C4-C5-N7	-3.66	106.39	110.58
3	C	500	ADP	N3-C4-N9	3.65	133.38	127.17
2	C	501	UDX	C5-C4-N3	3.64	119.90	114.80
2	E	502	UDX	C5-C4-N3	3.64	119.90	114.80
2	E	501	UDX	C5-C4-N3	3.55	119.78	114.80
3	F	500	ADP	C2-N3-C4	3.55	120.49	111.83
3	C	500	ADP	C4-N9-C8	3.54	109.45	105.74
2	D	501	UDX	C5-C4-N3	3.45	119.64	114.80
2	A	501	UDX	C5-C4-N3	3.44	119.61	114.80
2	A	502	UDX	O4-C4-C5	-3.42	119.27	125.16
2	E	502	UDX	O4-C4-C5	-3.38	119.33	125.16
2	F	501	UDX	O4-C4-C5	-3.34	119.39	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	UDX	O2-C2-N1	-3.31	118.48	122.80
2	A	502	UDX	O2-C2-N1	-3.21	118.62	122.80
3	C	500	ADP	C2-N3-C4	3.13	119.47	111.83
3	F	500	ADP	N3-C2-N1	-3.08	123.92	128.58
2	A	501	UDX	O4-C4-C5	-3.04	119.92	125.16
2	D	501	UDX	O4-C4-C5	-2.98	120.02	125.16
3	C	500	ADP	N3-C2-N1	-2.97	124.08	128.58
2	B	501	UDX	O3B-C1'-C2'	2.92	113.73	108.38
2	E	501	UDX	O4-C4-C5	-2.90	120.16	125.16
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	F	500	ADP	C4-N9-C8	2.74	108.62	105.74
3	F	500	ADP	C5-N7-C8	2.73	107.74	103.45
3	C	500	ADP	C5-N7-C8	2.65	107.62	103.45
3	C	500	ADP	N9-C8-N7	-2.63	110.21	113.94
2	E	502	UDX	O2-C2-N1	-2.62	119.38	122.80
3	C	500	ADP	C6-C5-N7	2.62	137.13	132.09
2	D	502	UDX	O2-C2-N1	-2.61	119.40	122.80
2	E	501	UDX	O3B-C1'-C2'	2.59	113.13	108.38
2	A	501	UDX	O2-C2-N1	-2.54	119.50	122.80
3	F	500	ADP	O2A-PA-O3A	2.52	114.07	107.27
2	C	501	UDX	O4-C4-C5	-2.51	120.83	125.16
3	F	500	ADP	C6-C5-N7	2.40	136.71	132.09
2	C	501	UDX	O2A-PA-O3A	2.37	113.67	107.27
2	D	502	UDX	O2A-PA-O3A	2.36	113.65	107.27
2	B	502	UDX	O4-C4-C5	-2.34	121.12	125.16
2	F	501	UDX	O2A-PA-O3A	2.33	113.58	107.27
2	B	501	UDX	C1'-C2'-C3'	2.28	114.81	110.01
2	B	502	UDX	O2-C2-N1	-2.25	119.87	122.80
3	F	500	ADP	N9-C8-N7	-2.24	110.75	113.94
2	B	501	UDX	O4-C4-C5	-2.24	121.31	125.16
2	D	501	UDX	C1D-N1-C2	2.23	121.60	117.59
2	C	501	UDX	O2'-C2'-C1'	-2.16	104.94	110.08
3	C	500	ADP	C4-N9-C1'	-2.07	121.78	126.63
3	F	500	ADP	O3A-PB-O1B	-2.06	100.22	111.04
2	A	502	UDX	O2A-PA-O3A	2.02	112.72	107.27

There are no chirality outliers.

All (22) torsion outliers are listed below:

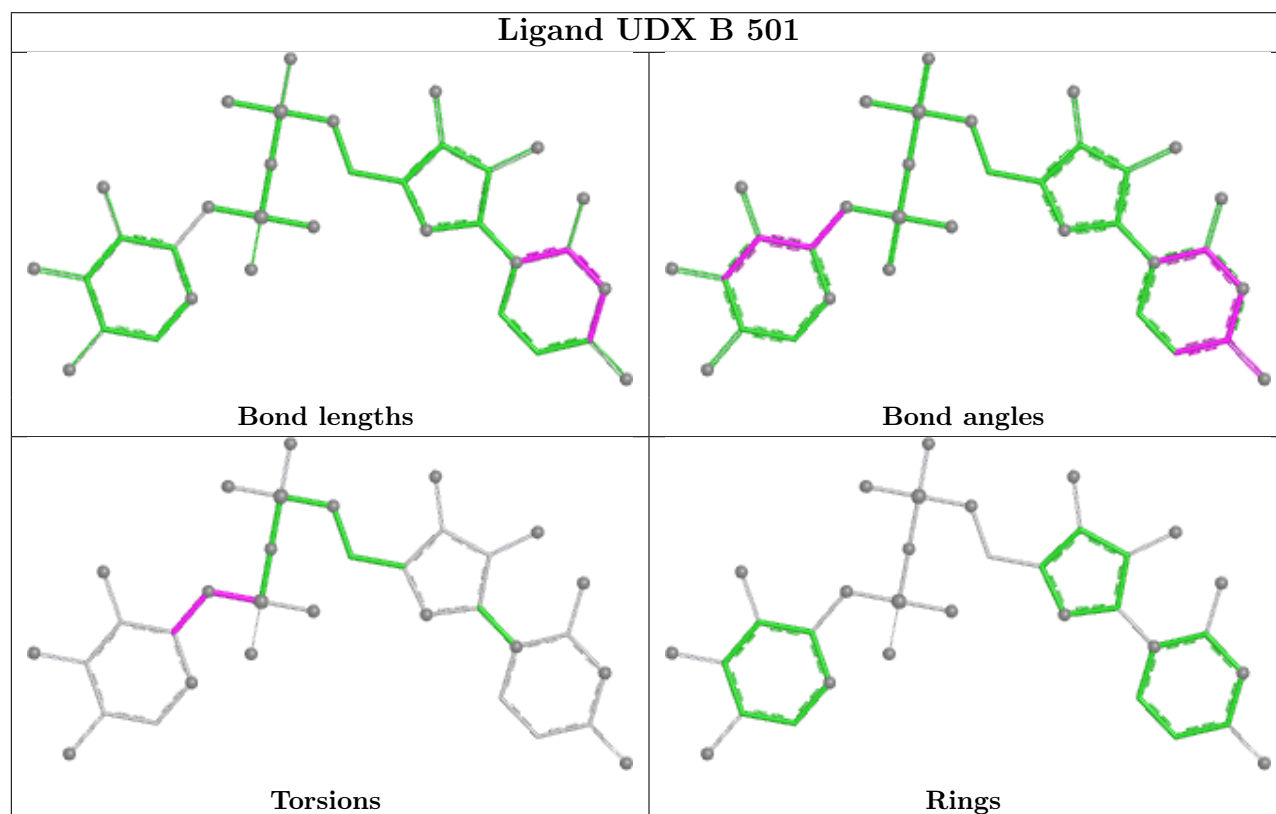
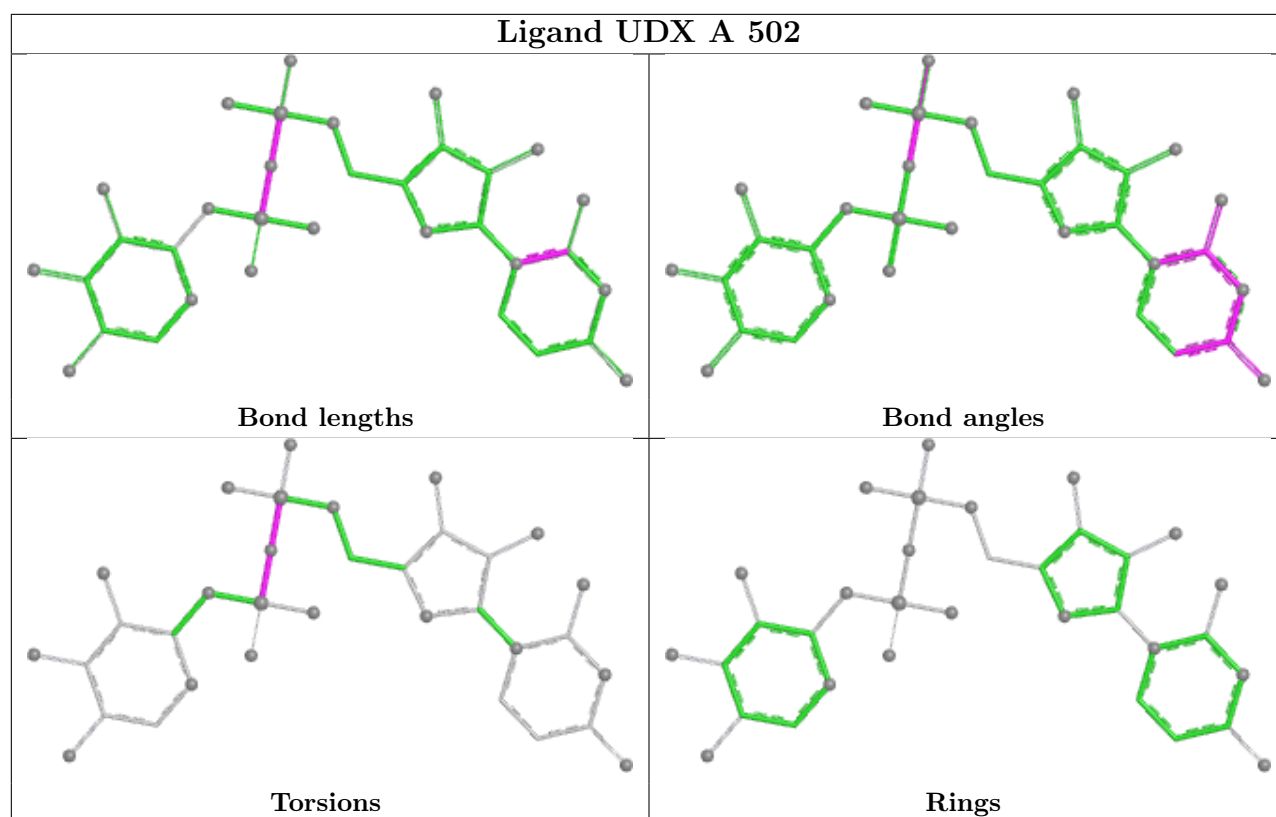
Mol	Chain	Res	Type	Atoms
2	A	501	UDX	C1'-O3B-PB-O2B
2	B	501	UDX	C1'-O3B-PB-O2B
2	B	501	UDX	C1'-O3B-PB-O3A
2	B	502	UDX	PA-O3A-PB-O3B
2	D	501	UDX	C1'-O3B-PB-O2B
2	E	501	UDX	C1'-O3B-PB-O2B
2	E	501	UDX	C1'-O3B-PB-O3A
2	A	502	UDX	PA-O3A-PB-O3B
2	C	501	UDX	PA-O3A-PB-O3B
2	D	502	UDX	PA-O3A-PB-O3B
2	B	501	UDX	C2'-C1'-O3B-PB
2	B	502	UDX	PB-O3A-PA-O1A
2	A	501	UDX	C2'-C1'-O3B-PB
2	D	501	UDX	C2'-C1'-O3B-PB
2	A	502	UDX	PB-O3A-PA-O1A
2	C	501	UDX	PB-O3A-PA-O1A
2	A	501	UDX	C1'-O3B-PB-O1B
2	D	501	UDX	C1'-O3B-PB-O1B
2	E	501	UDX	C1'-O3B-PB-O1B
3	F	500	ADP	O4'-C4'-C5'-O5'
3	C	500	ADP	O4'-C4'-C5'-O5'
2	E	501	UDX	C2'-C1'-O3B-PB

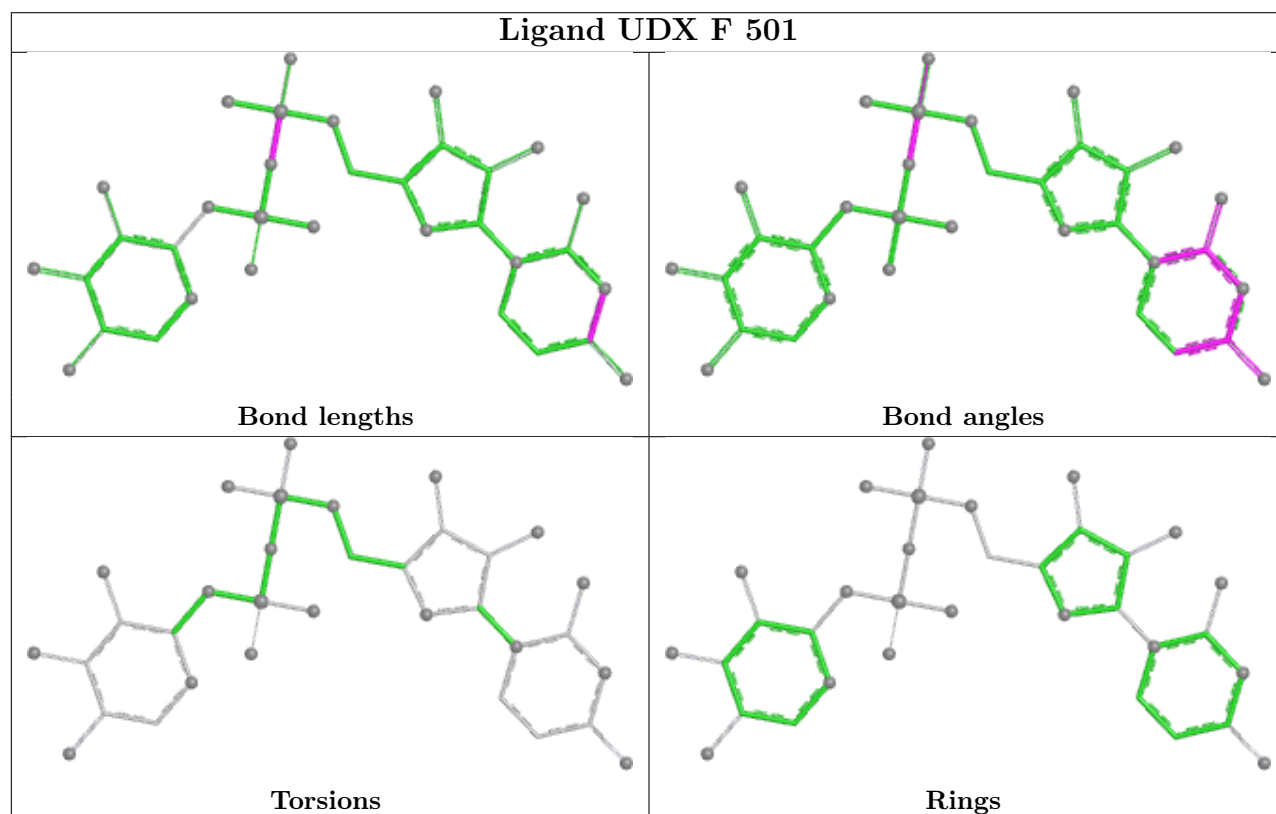
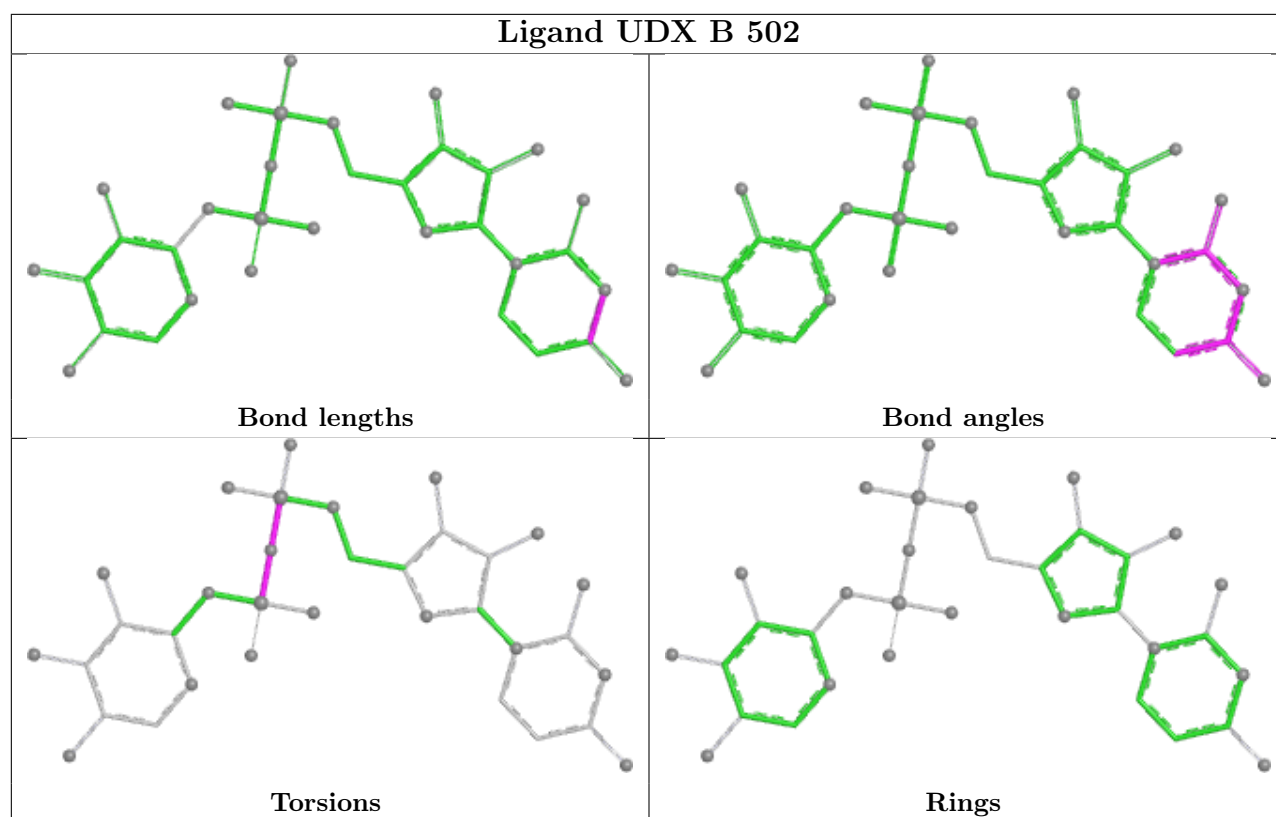
There are no ring outliers.

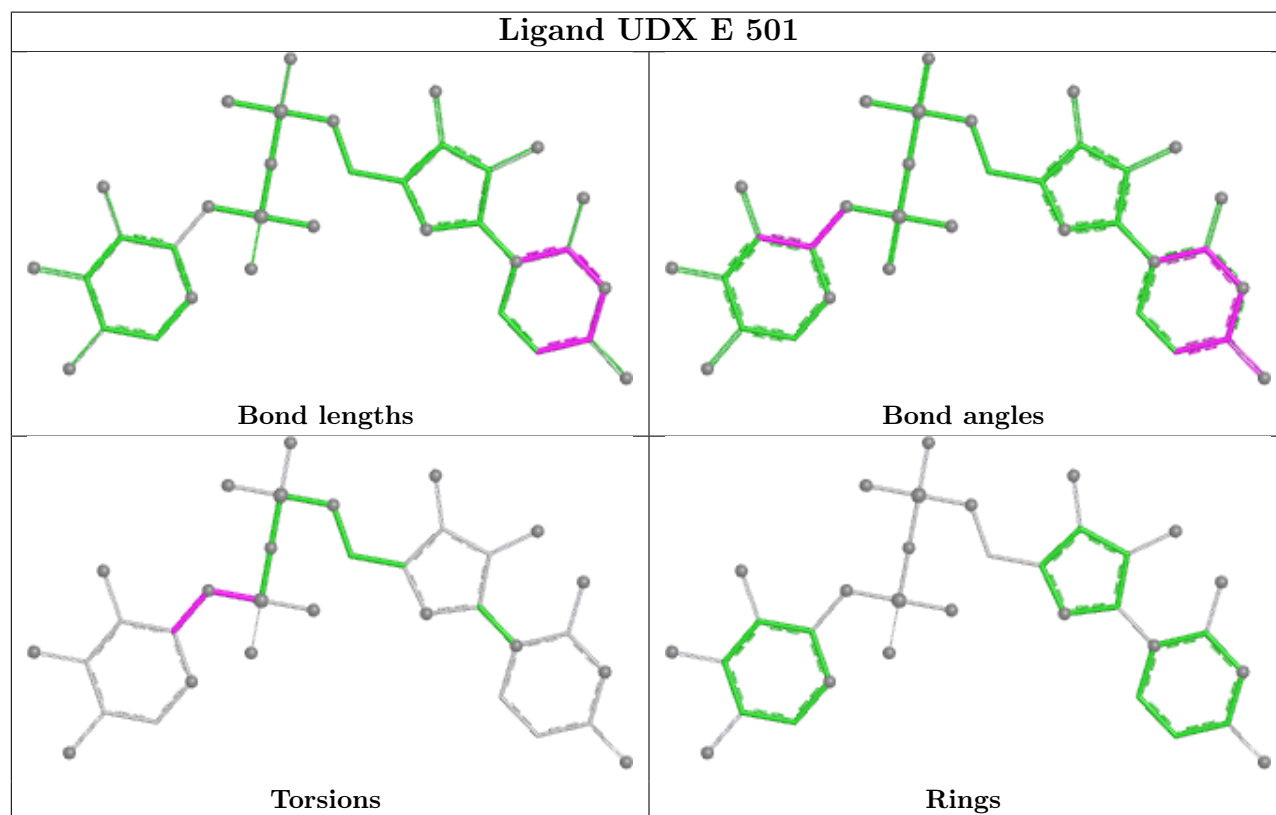
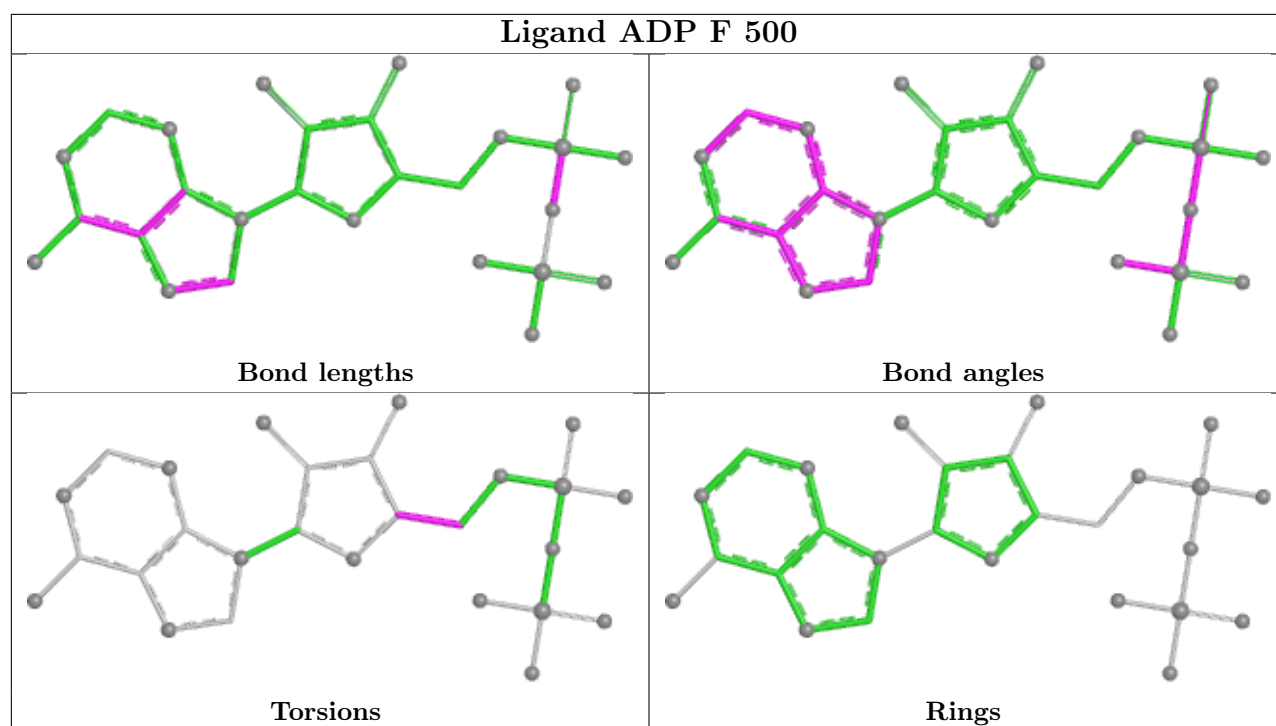
2 monomers are involved in 2 short contacts:

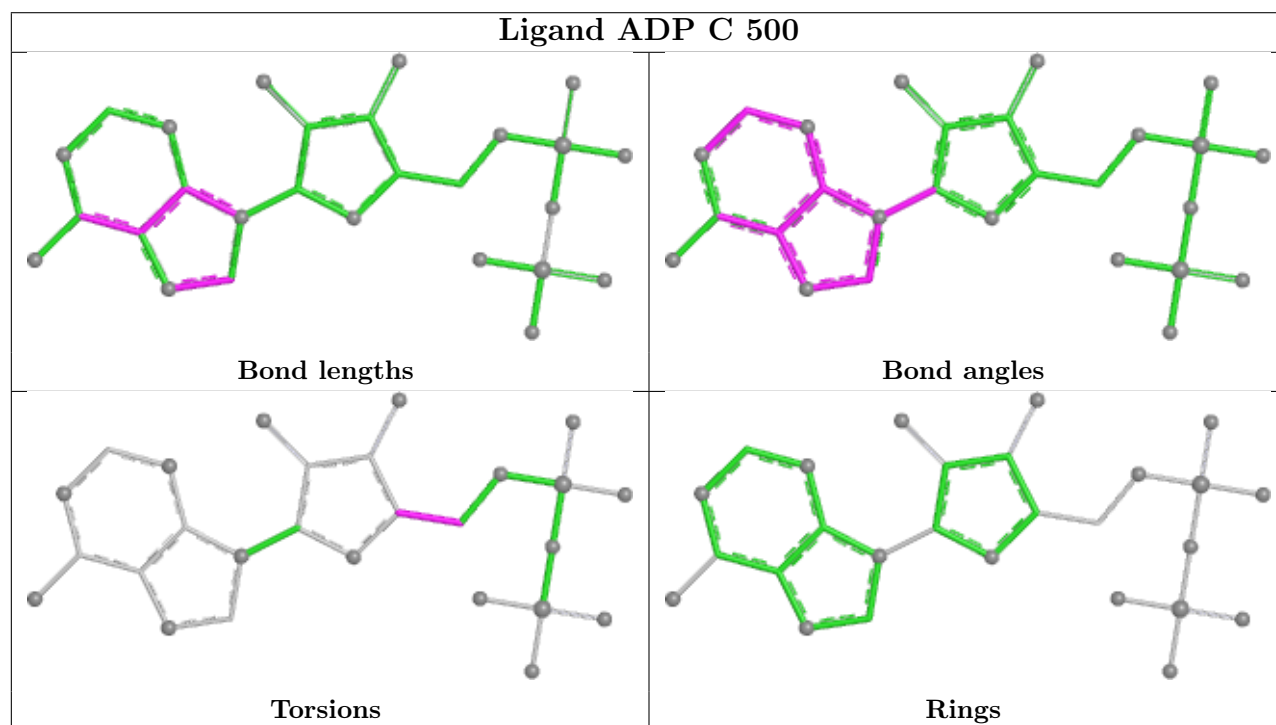
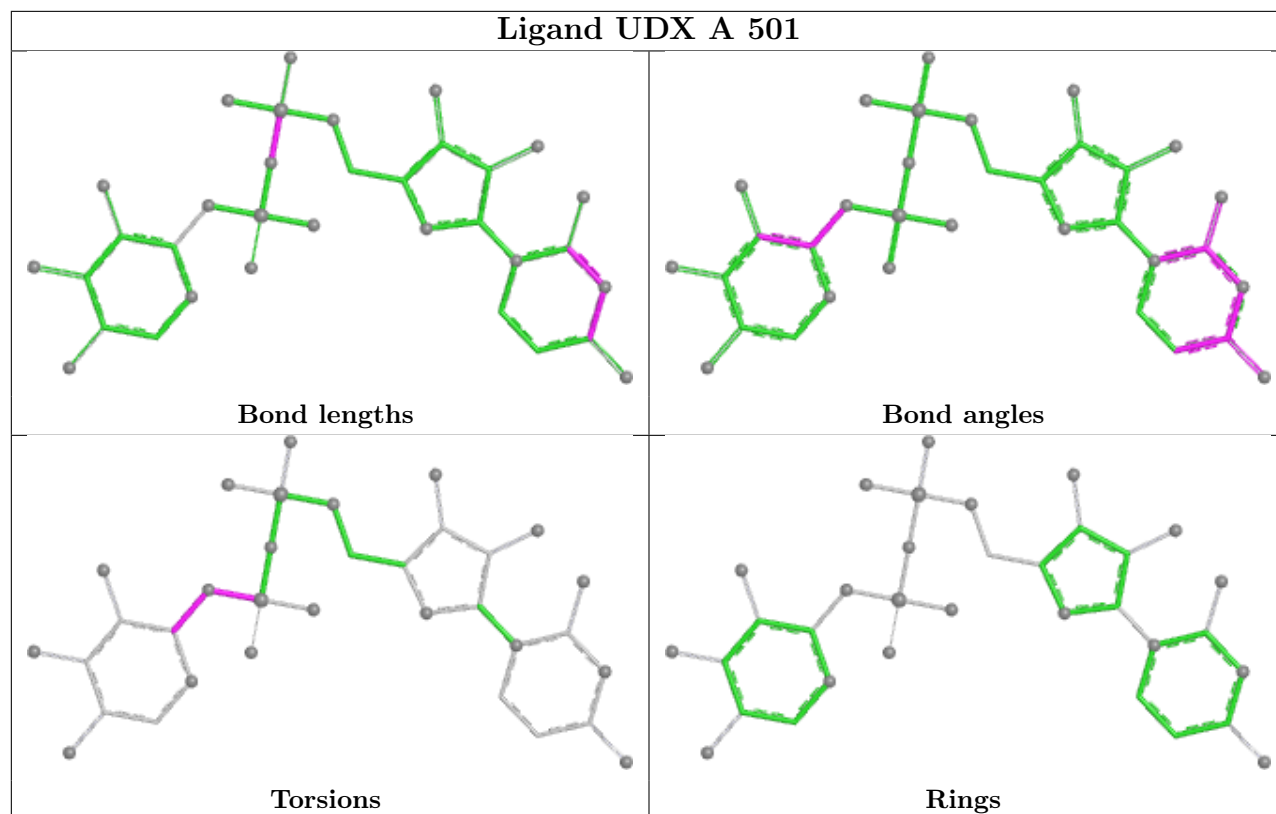
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	UDX	1	0
3	F	500	ADP	1	0

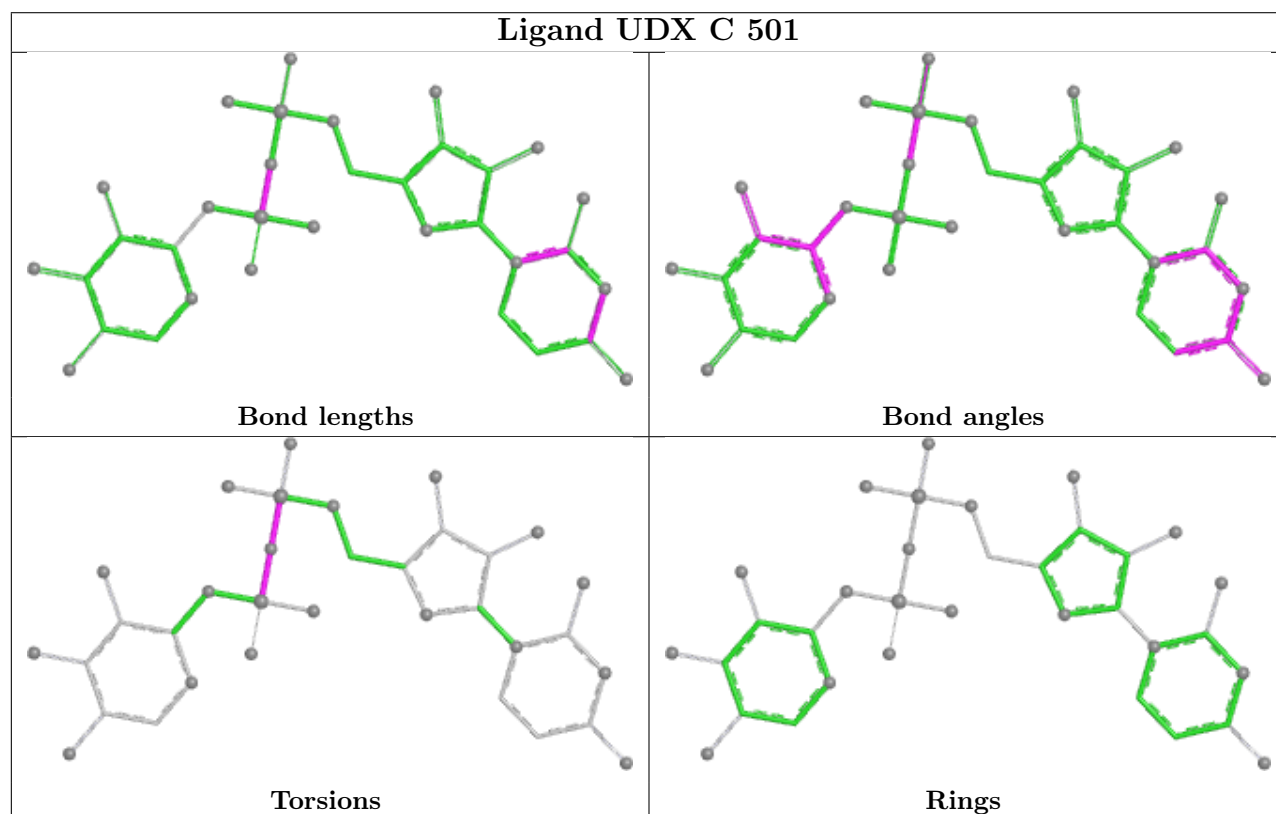
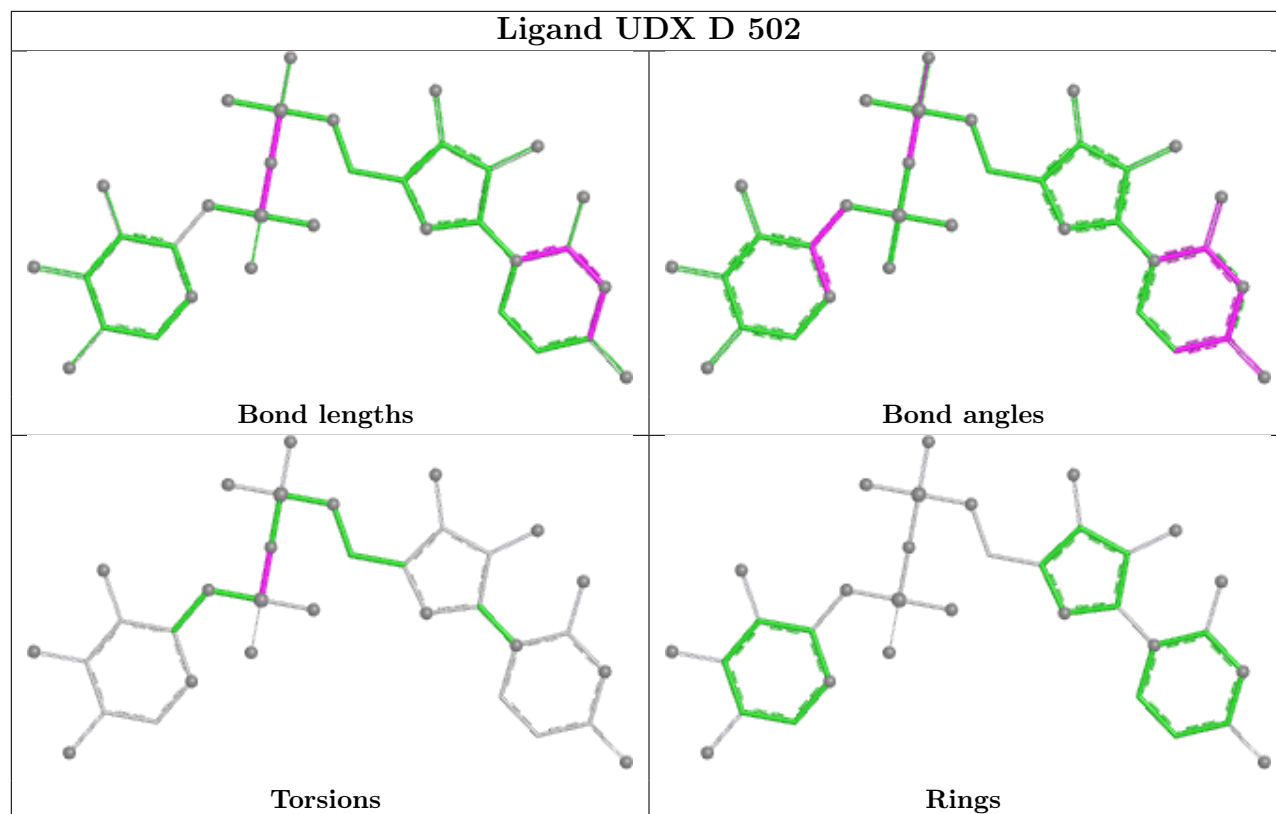
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

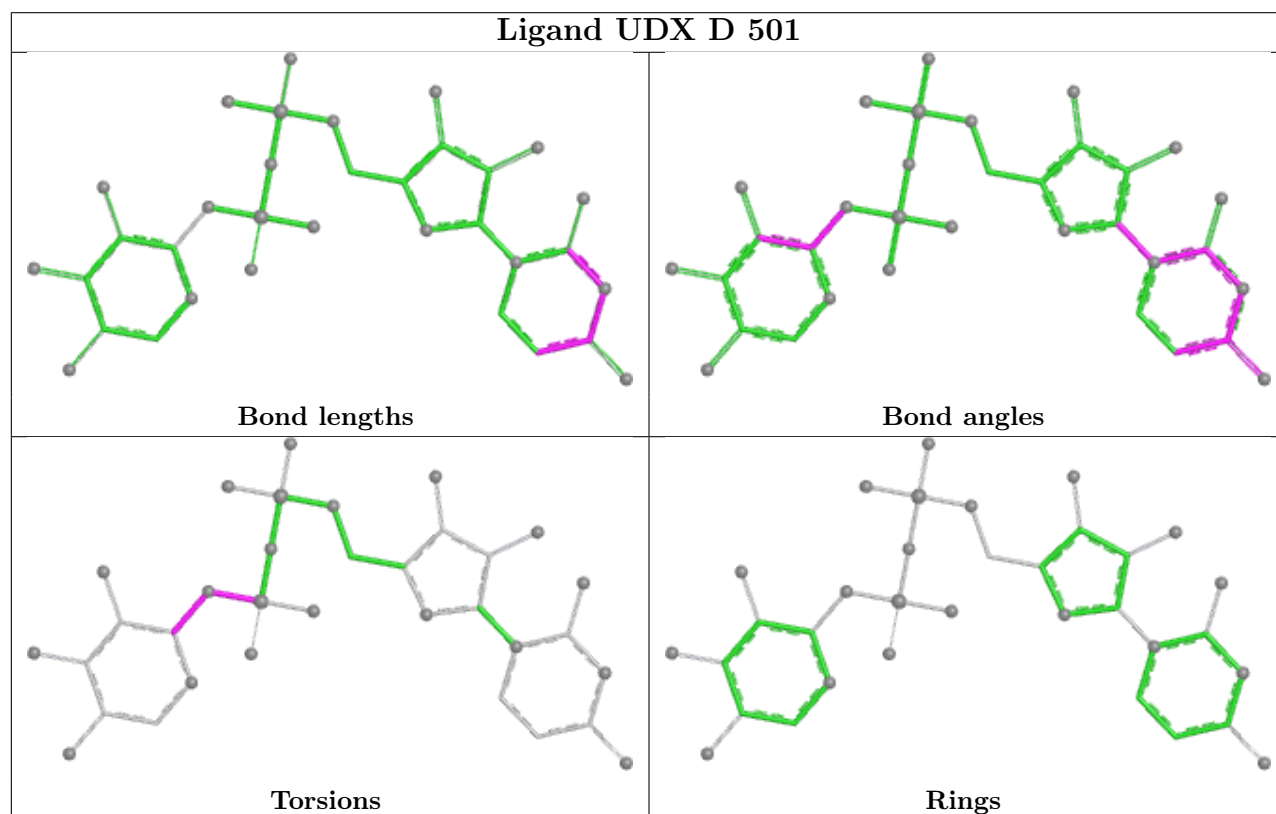
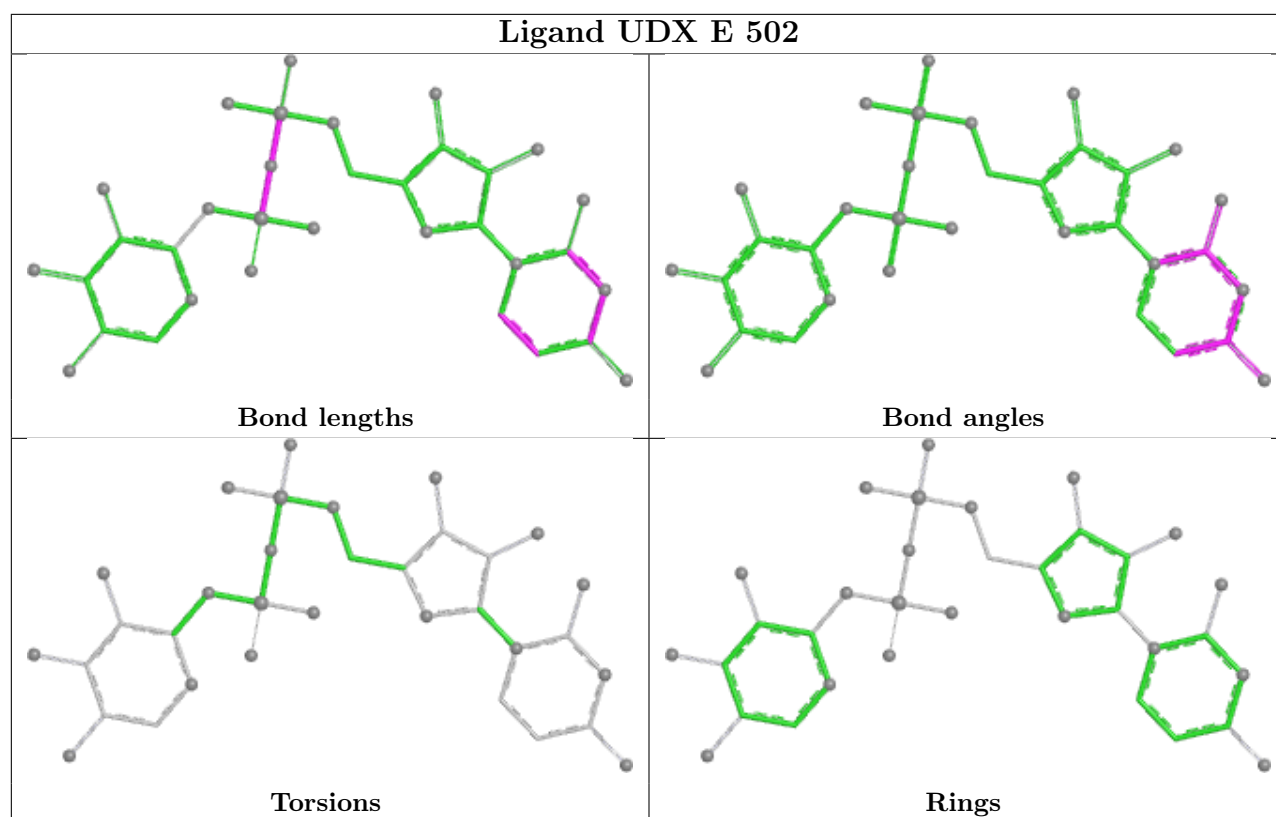












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	460/495 (92%)	-0.36	7 (1%) 72 71	16, 27, 47, 84	0
1	B	459/495 (92%)	-0.42	7 (1%) 72 71	15, 25, 45, 61	0
1	C	462/495 (93%)	-0.32	10 (2%) 62 61	17, 27, 53, 105	0
1	D	457/495 (92%)	-0.20	12 (2%) 57 56	19, 29, 63, 87	0
1	E	457/495 (92%)	-0.05	10 (2%) 62 61	18, 34, 67, 90	0
1	F	458/495 (92%)	-0.06	9 (1%) 65 64	19, 35, 57, 117	0
All	All	2753/2970 (92%)	-0.24	55 (1%) 65 64	15, 29, 57, 117	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	356	TYR	4.7
1	A	1	MET	4.6
1	C	465	LYS	4.6
1	C	98	MET	3.9
1	F	96	TYR	3.5
1	F	1	MET	3.5
1	C	0	HIS	3.5
1	C	96	TYR	3.3
1	D	98	MET	3.3
1	B	465	LYS	3.2
1	C	447	GLY	3.2
1	E	381	SER	3.2
1	E	389	ASP	3.0
1	A	459	ILE	3.0
1	B	447	GLY	2.9
1	A	465	LYS	2.9
1	F	98	MET	2.9
1	E	447	GLY	2.6
1	E	323	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	98	MET	2.6
1	A	388	ASP	2.6
1	B	98	MET	2.6
1	D	352	TYR	2.5
1	D	2	PHE	2.5
1	E	326	VAL	2.5
1	E	449	HIS	2.4
1	D	326	VAL	2.4
1	D	447	GLY	2.4
1	C	1	MET	2.4
1	E	465	LYS	2.4
1	D	454	THR	2.4
1	C	459	ILE	2.4
1	D	323	PHE	2.3
1	E	399	LYS	2.3
1	F	381	SER	2.3
1	F	389	ASP	2.3
1	C	382	HIS	2.3
1	F	447	GLY	2.2
1	F	465	LYS	2.2
1	B	64	CYS	2.2
1	D	389	ASP	2.2
1	B	323	PHE	2.2
1	A	98	MET	2.2
1	D	142	ARG	2.2
1	D	449	HIS	2.1
1	B	123	TYR	2.1
1	C	108	TYR	2.1
1	A	447	GLY	2.1
1	C	430	LYS	2.1
1	D	448	LEU	2.1
1	E	454	THR	2.0
1	F	93	THR	2.0
1	A	382	HIS	2.0
1	F	149	LYS	2.0
1	B	459	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

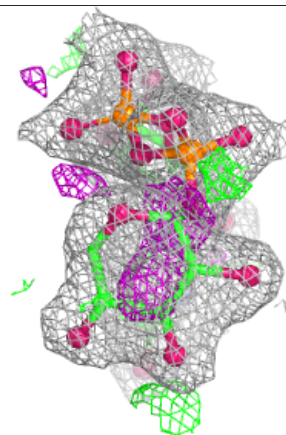
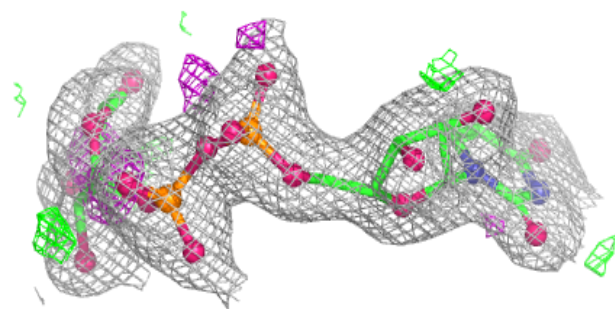
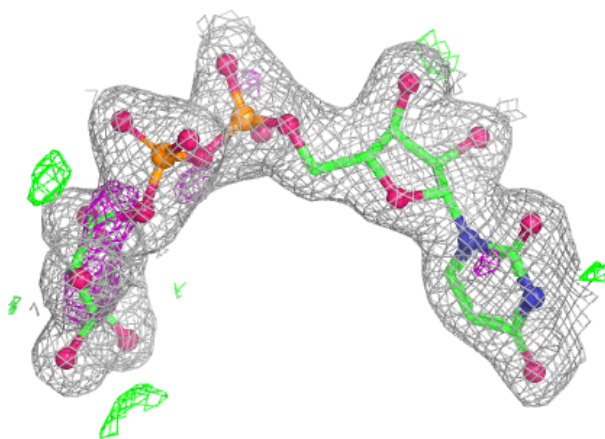
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UDX	E	501	34/34	0.96	0.08	27,36,54,56	0
2	UDX	D	501	34/34	0.97	0.08	19,29,51,52	0
2	UDX	A	501	34/34	0.97	0.07	22,30,47,48	0
3	ADP	F	500	27/27	0.97	0.07	31,39,47,54	0
2	UDX	E	502	34/34	0.98	0.04	18,22,25,29	0
3	ADP	C	500	27/27	0.98	0.06	24,29,43,46	0
2	UDX	B	501	34/34	0.98	0.06	18,26,44,46	0
2	UDX	B	502	34/34	0.99	0.04	14,17,19,20	0
2	UDX	C	501	34/34	0.99	0.03	15,18,22,23	0
2	UDX	F	501	34/34	0.99	0.04	19,22,26,28	0
2	UDX	A	502	34/34	0.99	0.04	15,19,21,23	0
2	UDX	D	502	34/34	0.99	0.04	17,22,24,27	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.

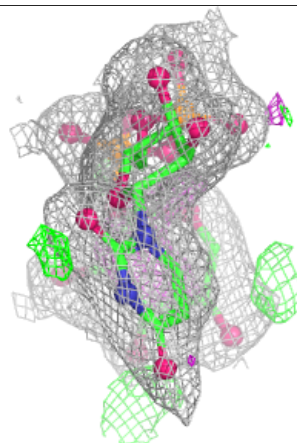
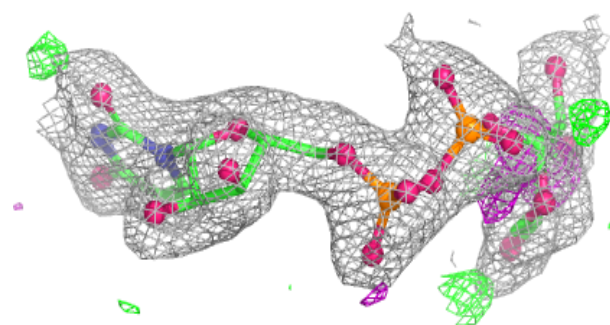
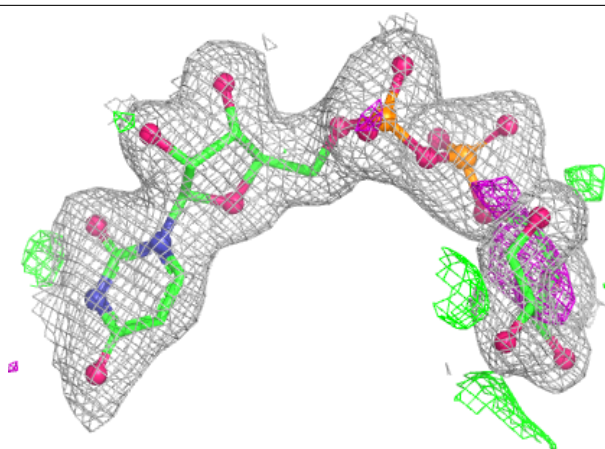
Electron density around UDX E 501:

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



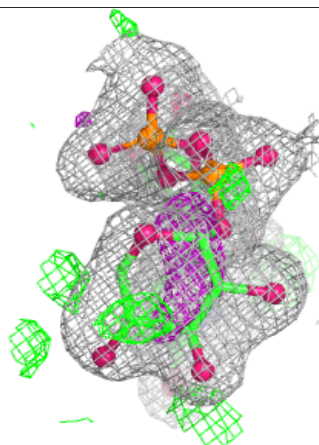
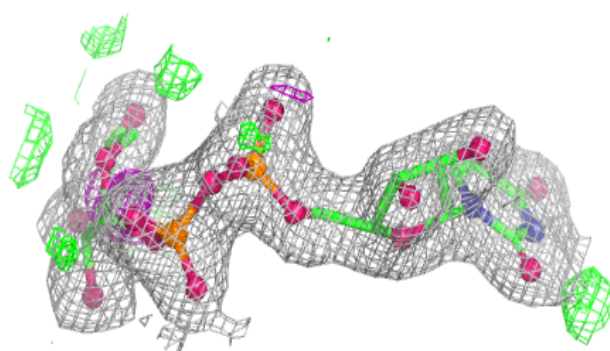
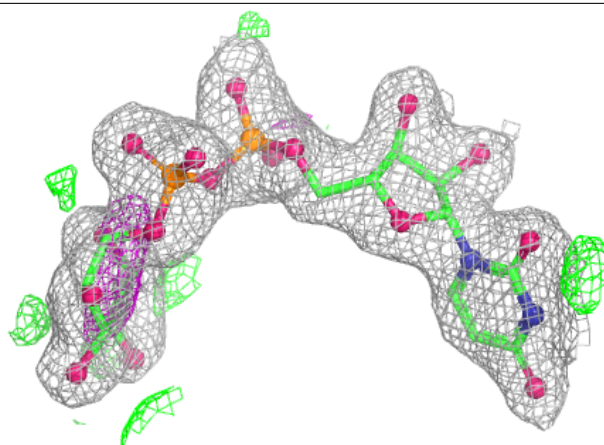
Electron density around UDX D 501:

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

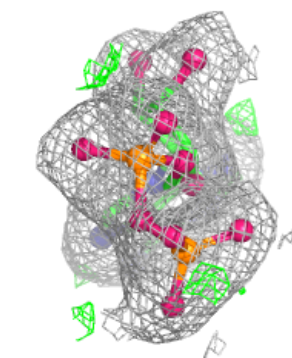
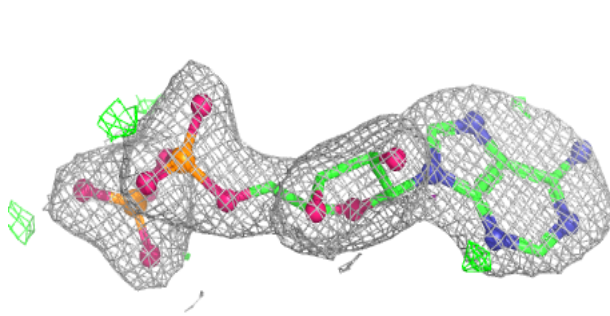
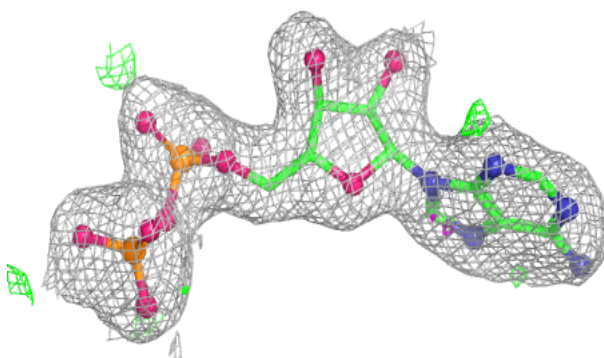


Electron density around UDX A 501:

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

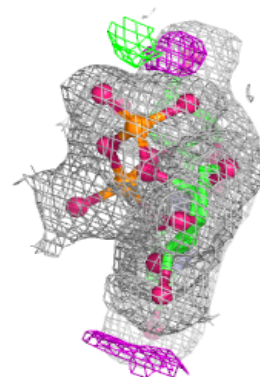
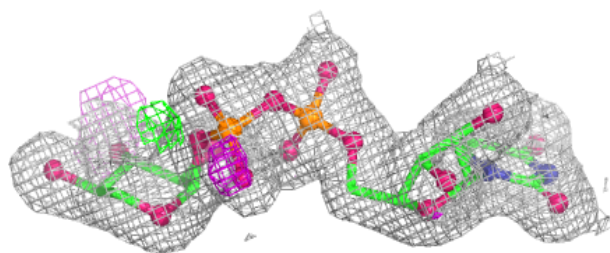
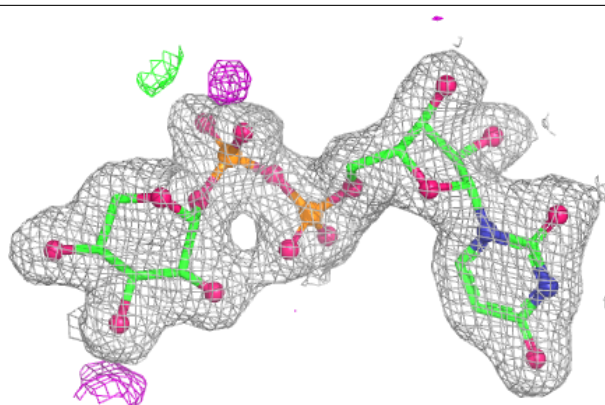
**Electron density around ADP F 500:**

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

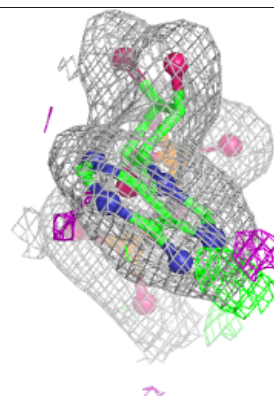
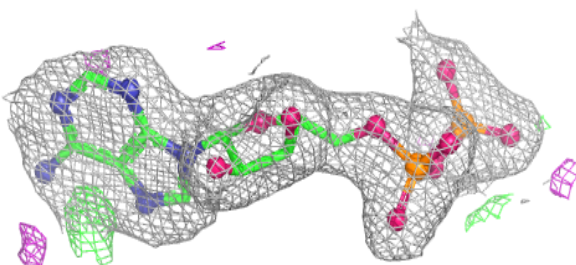
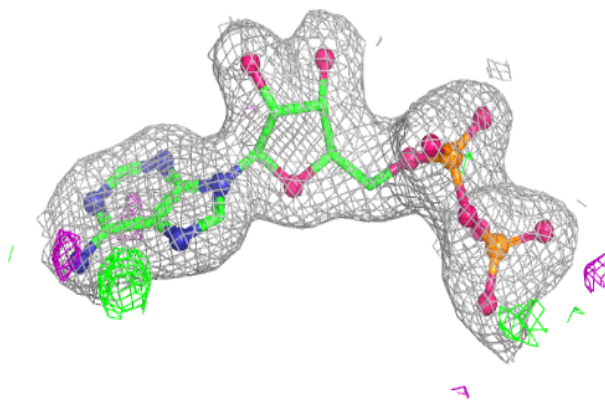


Electron density around UDX E 502:

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

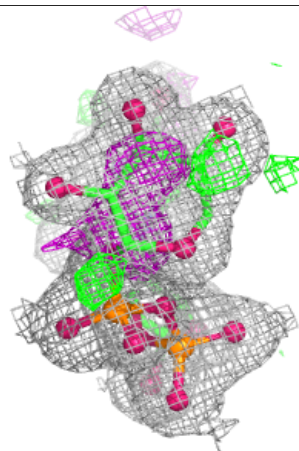
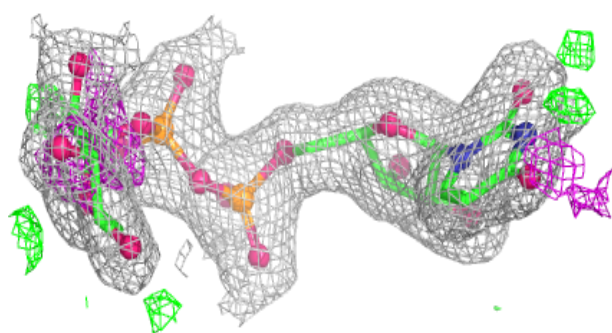
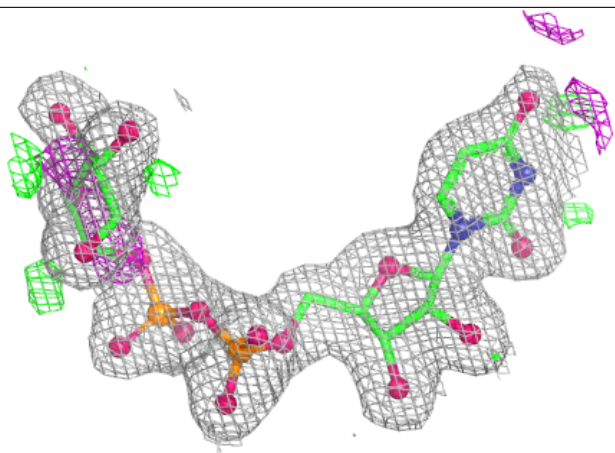
**Electron density around ADP C 500:**

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

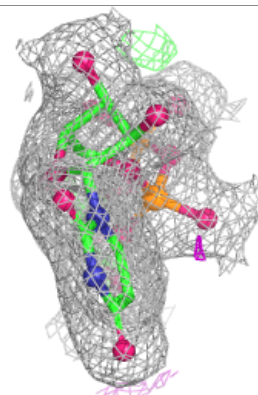
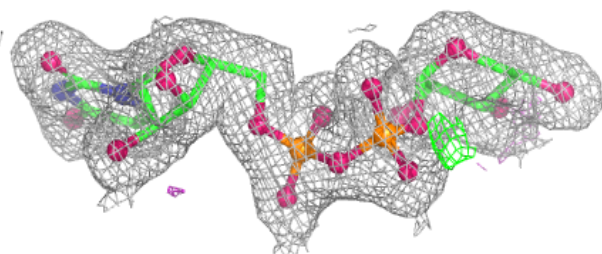
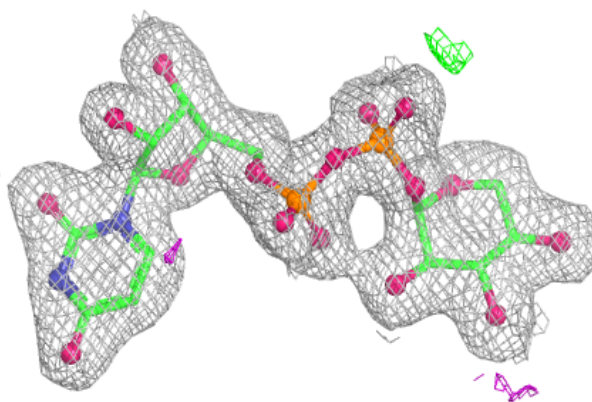


Electron density around UDX B 501:

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

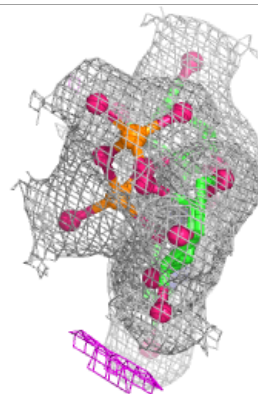
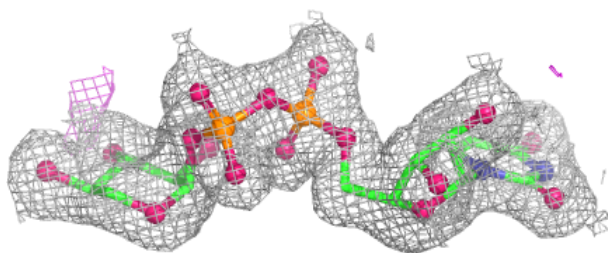
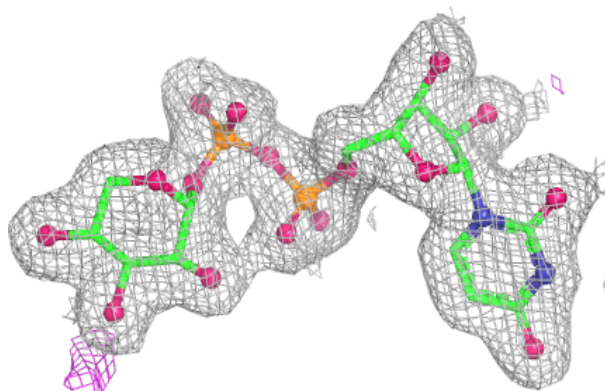
**Electron density around UDX B 502:**

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

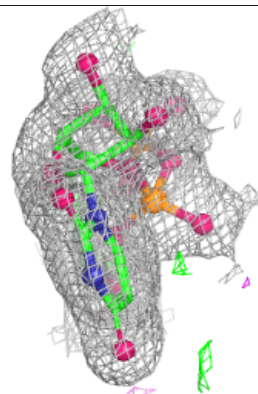
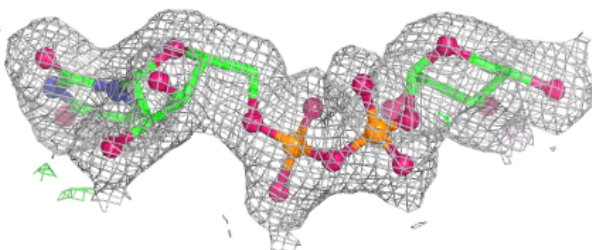
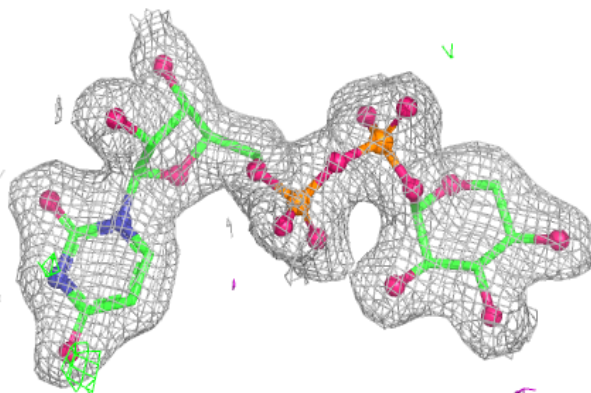


Electron density around UDX C 501:

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

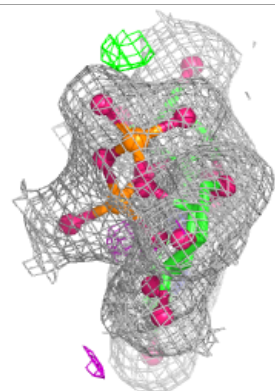
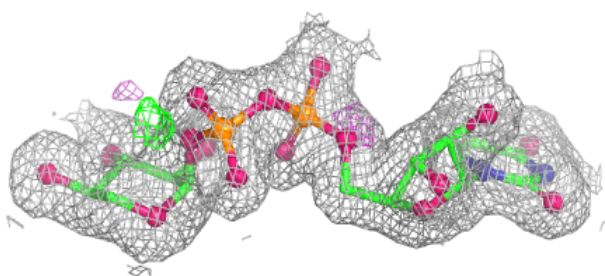
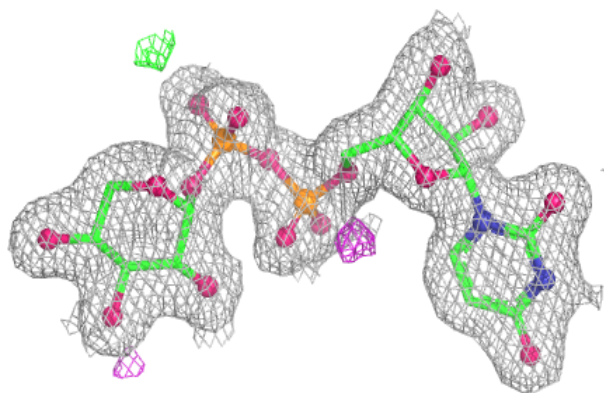
**Electron density around UDX F 501:**

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

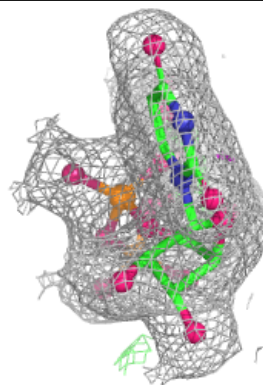
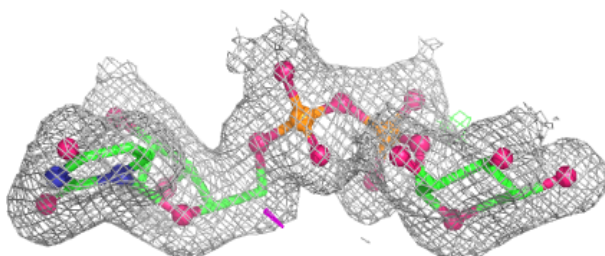
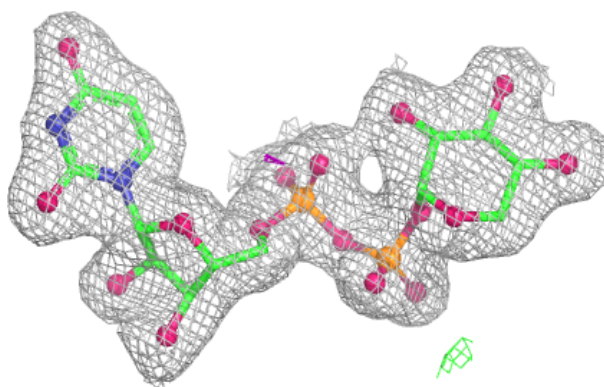


Electron density around UDX A 502:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.