



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:08 am BST

PDB ID : 6C58
Title : Human UDP-Glucose Dehydrogenase A225L substitutuion with UDP-xylose bound
Authors : Gross, P.G.; Fallah, J.; Wood, Z.A.
Deposited on : 2018-01-15
Resolution : 2.20 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

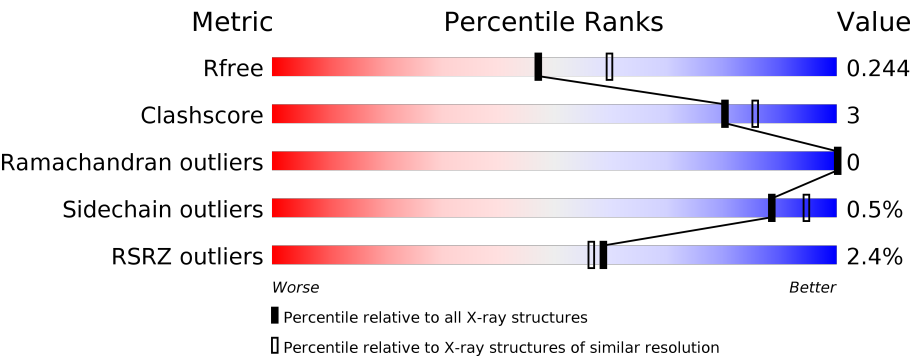
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	494	<div><div>%</div><div><div></div><div>86%</div><div>7%</div><div>7%</div></div></div>
1	B	494	<div><div>%</div><div><div></div><div>85%</div><div>8%</div><div>7%</div></div></div>
1	C	494	<div><div>%</div><div><div></div><div>87%</div><div>6%</div><div>7%</div></div></div>
1	D	494	<div><div>3%</div><div><div></div><div>85%</div><div>5%</div><div>9%</div></div></div>
1	E	494	<div><div>2%</div><div><div></div><div>85%</div><div>6%</div><div>10%</div></div></div>
1	F	494	<div><div>5%</div><div><div></div><div>89%</div><div>•</div><div>7%</div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22979 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.

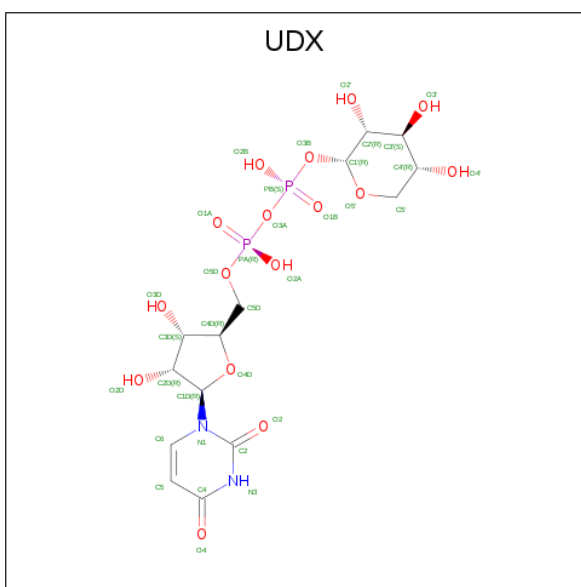
- Molecule 1 is a protein called UDP-glucose 6-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3617	2289	624	684	20			
1	B	459	Total	C	N	O	S	0	2	0
			3612	2287	625	680	20			
1	C	461	Total	C	N	O	S	0	0	0
			3618	2289	624	686	19			
1	D	449	Total	C	N	O	S	0	0	0
			3532	2236	607	671	18			
1	E	447	Total	C	N	O	S	0	0	0
			3515	2227	605	664	19			
1	F	459	Total	C	N	O	S	0	0	0
			3601	2280	622	680	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	LEU	ALA	engineered mutation	UNP O60701
B	225	LEU	ALA	engineered mutation	UNP O60701
C	225	LEU	ALA	engineered mutation	UNP O60701
D	225	LEU	ALA	engineered mutation	UNP O60701
E	225	LEU	ALA	engineered mutation	UNP O60701
F	225	LEU	ALA	engineered mutation	UNP O60701

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



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	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	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		
2	F	1	Total	C	N	O	P	0	0
			34	14	2	16	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Cl	0	0
			1	1		

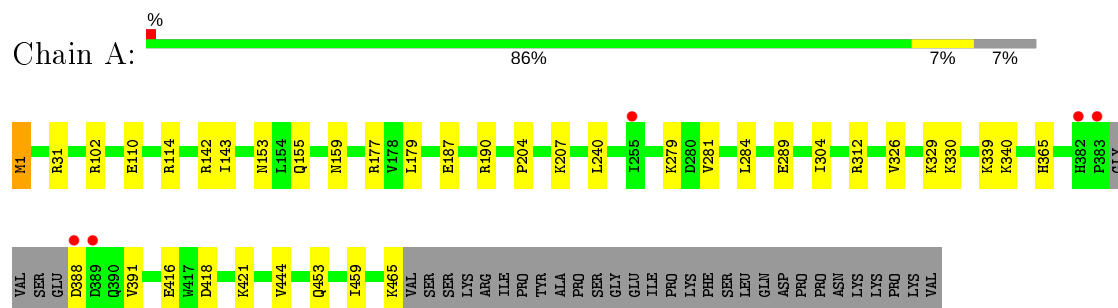
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	278	Total	O	0	0
			278	278		
4	B	212	Total	O	0	0
			212	212		
4	C	221	Total	O	0	0
			221	221		
4	D	125	Total	O	0	0
			125	125		
4	E	192	Total	O	0	0
			192	192		
4	F	113	Total	O	0	0
			113	113		

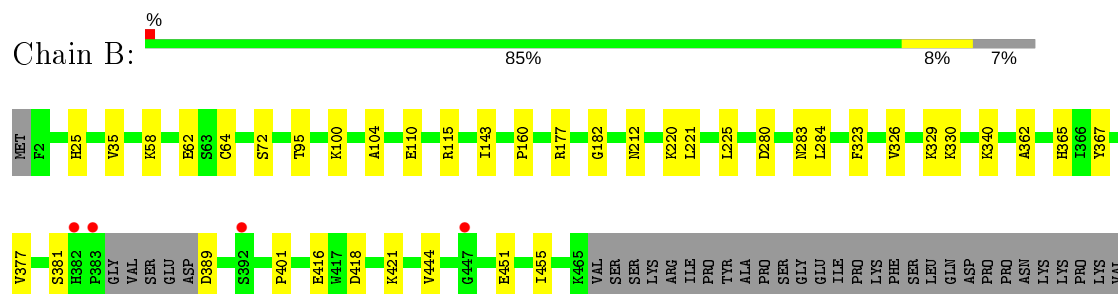
3 Residue-property plots [i](#)

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.

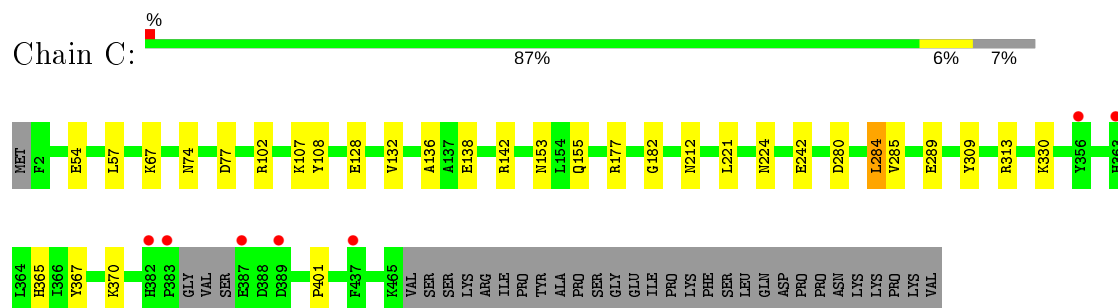
- Molecule 1: UDP-glucose 6-dehydrogenase



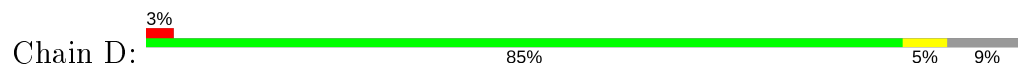
- Molecule 1: UDP-glucose 6-dehydrogenase

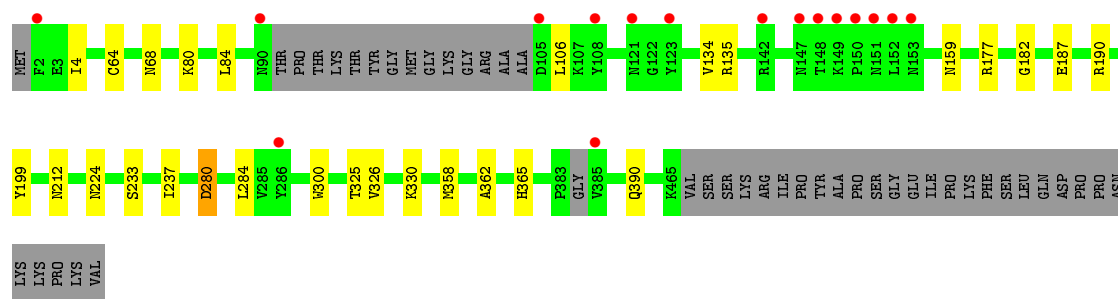


- Molecule 1: UDP-glucose 6-dehydrogenase

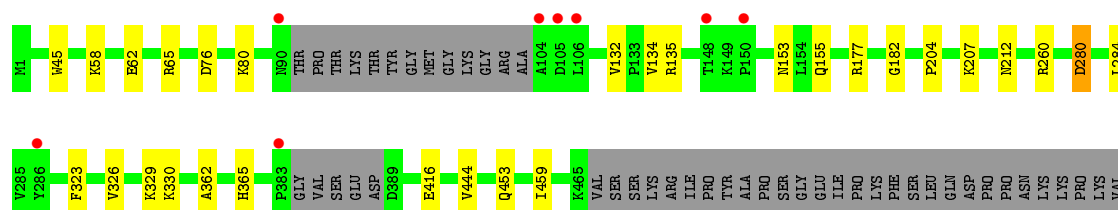
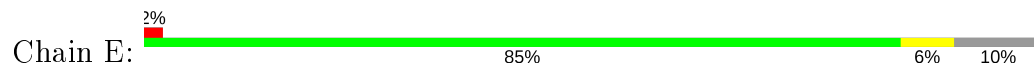


- Molecule 1: UDP-glucose 6-dehydrogenase

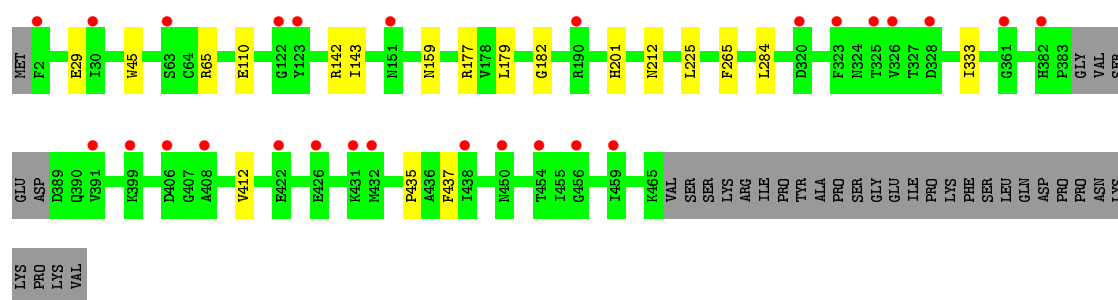
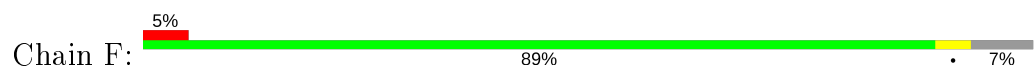




- Molecule 1: UDP-glucose 6-dehydrogenase



- Molecule 1: UDP-glucose 6-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.52Å 194.99Å 109.54Å 90.00° 110.71° 90.00°	Depositor
Resolution (Å)	51.29 – 2.20 51.29 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.4 (51.29-2.20) 86.3 (51.29-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.209 , 0.244 0.209 , 0.244	Depositor DCC
R_{free} test set	17886 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22979	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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, CL

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	0.39	0/3683	0.45	0/4983
1	B	0.34	0/3684	0.43	0/4984
1	C	0.25	0/3684	0.40	0/4985
1	D	0.30	0/3595	0.42	0/4865
1	E	0.38	0/3578	0.44	0/4841
1	F	0.31	0/3667	0.41	0/4962
All	All	0.33	0/21891	0.43	0/29620

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3617	0	3635	24	0
1	B	3612	0	3637	29	0
1	C	3618	0	3629	20	0
1	D	3532	0	3538	18	0
1	E	3515	0	3531	19	0
1	F	3601	0	3619	10	0
2	A	68	0	40	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	68	0	40	0	0
2	C	68	0	40	0	0
2	D	34	0	20	0	0
2	E	34	0	20	0	0
2	F	68	0	40	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	278	0	0	4	0
4	B	212	0	0	1	0
4	C	221	0	0	1	0
4	D	125	0	0	0	0
4	E	192	0	0	1	0
4	F	113	0	0	0	0
All	All	22979	0	21789	116	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 3.

All (116) 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:221:LEU:HD12	1:B:280:ASP:OD2	1.84	0.76
1:B:377:VAL:O	1:B:381:SER:OG	2.11	0.67
1:B:221:LEU:CD1	1:B:280:ASP:OD2	2.45	0.65
1:E:326:VAL:HG12	1:E:326:VAL:O	2.02	0.59
1:E:365:HIS:ND1	4:E:601:HOH:O	2.31	0.59
1:B:389:ASP:OD1	1:B:389:ASP:N	2.39	0.54
1:D:358:MET:CE	1:D:390:GLN:HG2	2.37	0.54
1:A:1:MET:HG2	1:A:190:ARG:HD3	1.89	0.54
1:A:281:VAL:HG11	1:A:304:ILE:HG12	1.87	0.54
1:A:187:GLU:OE1	1:A:190:ARG:NH2	2.37	0.54
1:A:284:LEU:HD13	1:A:284:LEU:C	2.28	0.54
1:D:325:THR:O	1:D:325:THR:HG23	2.08	0.53
1:F:333:ILE:HD13	1:F:412:VAL:HB	1.91	0.52
1:B:330:LYS:HE3	1:B:365:HIS:CG	2.45	0.52
1:C:102:ARG:NH1	1:C:289:GLU:OE1	2.43	0.52
1:A:142:ARG:HD3	1:E:323:PHE:HE1	1.75	0.52
1:C:221:LEU:HD11	1:C:284:LEU:HB2	1.92	0.52
1:F:45:TRP:O	1:F:65:ARG:NH1	2.41	0.52
1:B:326:VAL:CG1	1:B:362:ALA:HB2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:LEU:HD12	1:D:106:LEU:N	2.26	0.51
1:E:330:LYS:HE3	1:E:365:HIS:CG	2.46	0.51
1:D:159:ASN:ND2	1:D:199:TYR:OH	2.37	0.50
1:C:285:VAL:O	1:C:289:GLU:HG3	2.12	0.50
1:A:102:ARG:NH1	1:A:289:GLU:OE2	2.44	0.50
1:C:242:GLU:OE1	1:C:313:ARG:NH1	2.45	0.49
1:B:326:VAL:HG12	1:B:326:VAL:O	2.13	0.49
1:F:110:GLU:HG3	1:F:143:ILE:HD11	1.94	0.49
1:A:388:ASP:HB3	1:A:391:VAL:HB	1.96	0.48
1:A:153:ASN:OD1	1:A:155:GLN:NE2	2.46	0.48
1:A:453:GLN:HG3	1:A:459:ILE:HD13	1.96	0.48
1:B:115:ARG:NH1	4:B:610:HOH:O	2.38	0.48
1:B:340:LYS:HB3	1:B:416:GLU:HG2	1.96	0.48
1:A:159:ASN:ND2	1:A:179:LEU:O	2.40	0.48
1:C:128:GLU:HG3	1:C:136:ALA:HB1	1.94	0.47
1:A:240:LEU:HD11	1:B:284:LEU:HD21	1.95	0.47
1:E:134:VAL:HG22	1:E:135:ARG:HG3	1.97	0.47
1:F:159:ASN:ND2	1:F:179:LEU:O	2.40	0.47
1:A:340:LYS:HB3	1:A:416:GLU:HG2	1.97	0.47
1:F:29:GLU:OE2	1:F:201:HIS:NE2	2.46	0.47
1:D:134:VAL:HG22	1:D:135:ARG:HG3	1.96	0.47
1:C:67:LYS:NZ	4:C:613:HOH:O	2.45	0.47
1:E:204:PRO:HG2	1:E:207:LYS:HD2	1.96	0.47
1:B:182:GLY:O	1:B:212:ASN:HA	2.16	0.46
1:D:4:ILE:HD13	1:D:84:LEU:HB2	1.96	0.46
1:C:242:GLU:CD	1:C:313:ARG:HH12	2.18	0.46
1:E:330:LYS:HE3	1:E:365:HIS:CD2	2.51	0.46
1:A:312:ARG:NH2	4:A:607:HOH:O	2.42	0.46
1:B:367:TYR:CE2	1:B:401:PRO:HG3	2.51	0.46
1:C:138:GLU:O	1:C:142:ARG:HG2	2.16	0.46
1:A:330:LYS:HE3	1:A:365:HIS:CG	2.50	0.46
1:C:284:LEU:C	1:C:284:LEU:HD13	2.37	0.45
1:D:182:GLY:O	1:D:212:ASN:HA	2.17	0.45
1:D:326:VAL:CG1	1:D:362:ALA:HB2	2.47	0.45
1:E:284:LEU:C	1:E:284:LEU:HD13	2.36	0.45
1:C:74:ASN:ND2	1:C:77:ASP:OD2	2.44	0.45
1:B:225:LEU:HD11	1:B:284:LEU:HG	1.99	0.44
1:A:204:PRO:HD2	1:A:207:LYS:HD3	1.99	0.44
1:A:330:LYS:HE3	1:A:365:HIS:CD2	2.52	0.44
1:A:416:GLU:HA	1:A:444:VAL:HG11	1.99	0.44
1:A:418:ASP:O	1:A:421:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:GLU:HA	1:E:444:VAL:HG11	2.00	0.44
1:E:58:LYS:NZ	1:E:62:GLU:OE2	2.35	0.44
1:B:418:ASP:O	1:B:421:LYS:HG2	2.17	0.44
1:C:107:LYS:HE3	1:C:108:TYR:CZ	2.53	0.44
1:C:54:GLU:HB3	1:C:57:LEU:HB2	2.00	0.44
1:D:330:LYS:HE3	1:D:365:HIS:CD2	2.53	0.44
1:A:326:VAL:HA	1:A:329:LYS:HD2	1.99	0.44
1:A:279:LYS:NZ	4:A:604:HOH:O	2.36	0.43
1:A:114:ARG:NH2	4:A:616:HOH:O	2.45	0.43
1:D:326:VAL:HG12	1:D:326:VAL:O	2.18	0.43
1:B:160:PRO:HB3	1:B:220:LYS:HG2	2.00	0.43
1:F:182:GLY:O	1:F:212:ASN:HA	2.18	0.43
1:C:153:ASN:OD1	1:C:155:GLN:NE2	2.52	0.42
1:C:224:ASN:HB2	1:C:280:ASP:OD2	2.19	0.42
1:E:260:ARG:HD2	1:F:265:PHE:CE1	2.54	0.42
1:C:367:TYR:CE2	1:C:401:PRO:HG3	2.54	0.42
1:D:330:LYS:HE3	1:D:365:HIS:CG	2.54	0.42
1:C:330:LYS:HE3	1:C:365:HIS:CG	2.55	0.42
1:E:76:ASP:O	1:E:80:LYS:HG3	2.19	0.42
1:B:110:GLU:HG3	1:B:143:ILE:HD11	2.02	0.42
1:B:323:PHE:HE1	1:F:142:ARG:HD2	1.84	0.42
1:B:416:GLU:HA	1:B:444:VAL:HG11	2.02	0.42
1:C:132:VAL:HG13	1:C:280:ASP:OD1	2.19	0.42
1:F:225:LEU:HD11	1:F:284:LEU:HD22	2.02	0.42
1:A:31:ARG:NH2	4:A:624:HOH:O	2.49	0.42
1:E:453:GLN:HG3	1:E:459:ILE:HD13	2.01	0.42
1:C:309:TYR:CZ	1:C:313:ARG:HD3	2.54	0.42
1:C:370:LYS:HD3	1:C:370:LYS:HA	1.88	0.42
1:E:182:GLY:O	1:E:212:ASN:HA	2.20	0.42
1:A:110:GLU:HG3	1:A:143:ILE:HD11	2.01	0.41
1:B:330:LYS:HE3	1:B:365:HIS:CD2	2.56	0.41
1:D:284:LEU:HD12	1:D:300:TRP:HB2	2.02	0.41
1:D:80:LYS:HE3	1:D:80:LYS:HB2	1.80	0.41
1:B:104:ALA:HB2	1:B:283:ASN:HD21	1.84	0.41
1:E:132:VAL:HG13	1:E:280:ASP:OD1	2.20	0.41
1:B:326:VAL:HG12	1:B:362:ALA:HB2	2.02	0.41
1:D:187:GLU:OE1	1:D:190:ARG:NH2	2.53	0.41
1:B:35:VAL:HA	1:B:72:SER:O	2.20	0.41
1:C:182:GLY:O	1:C:212:ASN:HA	2.21	0.41
1:E:153:ASN:OD1	1:E:155:GLN:NE2	2.54	0.41
1:F:435:PRO:HG2	1:F:437:PHE:HE1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:THR:O	1:B:100:LYS:NZ	2.47	0.41
1:D:224:ASN:ND2	1:D:280:ASP:OD2	2.40	0.41
1:E:326:VAL:HG11	1:E:362:ALA:HB2	2.03	0.41
1:A:339:LYS:NZ	2:A:502:UDX:O1A	2.35	0.41
1:E:326:VAL:HA	1:E:329:LYS:HD2	2.02	0.41
1:B:326:VAL:HA	1:B:329:LYS:HD2	2.03	0.41
1:B:451:GLU:O	1:B:455:ILE:HG13	2.21	0.41
1:D:358:MET:HE3	1:D:390:GLN:HG2	2.03	0.41
1:B:25:HIS:HA	1:B:64[B]:CYS:SG	2.60	0.40
1:D:233:SER:O	1:D:237:ILE:HG12	2.21	0.40
1:D:64:CYS:HB2	1:D:68:ASN:OD1	2.21	0.40
1:B:421:LYS:HE2	1:B:421:LYS:HB3	1.98	0.40
1:B:326:VAL:HG11	1:B:362:ALA:HB2	2.02	0.40
1:B:58:LYS:NZ	1:B:62:GLU:OE2	2.52	0.40
1:E:45:TRP:O	1:E:65:ARG:NH1	2.53	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	457/494 (92%)	445 (97%)	12 (3%)	0	100	100
1	B	457/494 (92%)	442 (97%)	15 (3%)	0	100	100
1	C	457/494 (92%)	446 (98%)	11 (2%)	0	100	100
1	D	443/494 (90%)	431 (97%)	12 (3%)	0	100	100
1	E	441/494 (89%)	433 (98%)	8 (2%)	0	100	100
1	F	455/494 (92%)	437 (96%)	18 (4%)	0	100	100
All	All	2710/2964 (91%)	2634 (97%)	76 (3%)	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	397/427 (93%)	394 (99%)	3 (1%)	81	90
1	B	397/427 (93%)	396 (100%)	1 (0%)	92	97
1	C	397/427 (93%)	395 (100%)	2 (0%)	88	94
1	D	390/427 (91%)	388 (100%)	2 (0%)	88	94
1	E	387/427 (91%)	385 (100%)	2 (0%)	88	94
1	F	395/427 (92%)	394 (100%)	1 (0%)	92	97
All	All	2363/2562 (92%)	2352 (100%)	11 (0%)	88	94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	177	ARG
1	A	465	LYS
1	B	177	ARG
1	C	177	ARG
1	C	284	LEU
1	D	177	ARG
1	D	280	ASP
1	E	177	ARG
1	E	280	ASP
1	F	177	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	ASN
1	B	283	ASN
1	D	159	ASN
1	E	155	GLN
1	E	283	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	UDX	F	501	-	29,36,36	1.12	3 (10%)	38,55,55	1.16	3 (7%)
2	UDX	B	502	-	29,36,36	1.14	3 (10%)	38,55,55	1.10	2 (5%)
2	UDX	C	500	-	29,36,36	1.13	3 (10%)	38,55,55	1.18	2 (5%)
2	UDX	C	501	-	29,36,36	1.15	3 (10%)	38,55,55	1.11	2 (5%)
2	UDX	A	501	-	29,36,36	1.12	3 (10%)	38,55,55	1.25	3 (7%)
2	UDX	D	501	-	29,36,36	1.12	3 (10%)	38,55,55	1.14	2 (5%)
2	UDX	B	501	-	29,36,36	1.09	3 (10%)	38,55,55	1.21	2 (5%)
2	UDX	E	501	-	29,36,36	1.12	3 (10%)	38,55,55	1.14	2 (5%)
2	UDX	F	500	-	29,36,36	1.14	3 (10%)	38,55,55	1.27	3 (7%)
2	UDX	A	502	-	29,36,36	1.14	3 (10%)	38,55,55	1.10	2 (5%)

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	F	501	-	-	2/19/54/54	0/3/3/3
2	UDX	B	502	-	-	4/19/54/54	0/3/3/3
2	UDX	C	500	-	-	6/19/54/54	0/3/3/3
2	UDX	C	501	-	-	4/19/54/54	0/3/3/3
2	UDX	A	501	-	-	6/19/54/54	0/3/3/3
2	UDX	D	501	-	-	4/19/54/54	0/3/3/3
2	UDX	B	501	-	-	6/19/54/54	0/3/3/3
2	UDX	E	501	-	-	4/19/54/54	0/3/3/3
2	UDX	F	500	-	-	6/19/54/54	0/3/3/3
2	UDX	A	502	-	-	4/19/54/54	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	UDX	C4-N3	3.23	1.38	1.33
2	D	501	UDX	C4-N3	3.23	1.38	1.33
2	B	502	UDX	C4-N3	3.22	1.38	1.33
2	C	500	UDX	C4-N3	3.19	1.38	1.33
2	A	502	UDX	C4-N3	3.18	1.38	1.33
2	F	500	UDX	C4-N3	3.18	1.38	1.33
2	F	501	UDX	C4-N3	3.17	1.38	1.33
2	C	501	UDX	C4-N3	3.16	1.38	1.33
2	A	501	UDX	C4-N3	3.13	1.38	1.33
2	B	501	UDX	C4-N3	3.04	1.38	1.33
2	C	501	UDX	O4D-C1D	3.00	1.45	1.41
2	A	502	UDX	O4D-C1D	2.97	1.45	1.41
2	C	500	UDX	O4D-C1D	2.93	1.45	1.41
2	B	502	UDX	O4D-C1D	2.93	1.45	1.41
2	E	501	UDX	O4D-C1D	2.88	1.45	1.41
2	F	501	UDX	O4D-C1D	2.87	1.45	1.41
2	F	500	UDX	O4D-C1D	2.84	1.45	1.41
2	A	501	UDX	O4D-C1D	2.82	1.45	1.41
2	D	501	UDX	O4D-C1D	2.81	1.45	1.41
2	A	501	UDX	C6-C5	-2.70	1.32	1.38
2	F	500	UDX	C6-C5	-2.69	1.32	1.38
2	C	501	UDX	C6-C5	-2.68	1.32	1.38
2	B	501	UDX	C6-C5	-2.67	1.32	1.38
2	E	501	UDX	C6-C5	-2.65	1.32	1.38
2	A	502	UDX	C6-C5	-2.65	1.32	1.38
2	B	502	UDX	C6-C5	-2.64	1.32	1.38
2	B	501	UDX	O4D-C1D	2.64	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	UDX	C6-C5	-2.64	1.32	1.38
2	F	501	UDX	C6-C5	-2.61	1.32	1.38
2	C	500	UDX	C6-C5	-2.59	1.32	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	UDX	C5-C4-N3	-4.14	114.19	123.31
2	C	500	UDX	C5-C4-N3	-4.14	114.20	123.31
2	B	502	UDX	C5-C4-N3	-4.12	114.25	123.31
2	E	501	UDX	C5-C4-N3	-4.11	114.26	123.31
2	F	500	UDX	C5-C4-N3	-4.11	114.26	123.31
2	A	502	UDX	C5-C4-N3	-4.11	114.27	123.31
2	A	501	UDX	C5-C4-N3	-4.08	114.34	123.31
2	B	501	UDX	C5-C4-N3	-4.06	114.37	123.31
2	D	501	UDX	C5-C4-N3	-4.04	114.41	123.31
2	C	501	UDX	C5-C4-N3	-4.01	114.49	123.31
2	F	500	UDX	O3A-PB-O3B	2.83	108.20	102.48
2	D	501	UDX	O3A-PB-O3B	2.71	107.95	102.48
2	F	501	UDX	O3A-PB-O3B	2.44	107.40	102.48
2	E	501	UDX	O3A-PB-O3B	2.38	107.28	102.48
2	A	501	UDX	C5'-O5'-C1'	2.32	117.06	112.38
2	B	501	UDX	C5'-O5'-C1'	2.24	116.90	112.38
2	A	502	UDX	O3A-PB-O3B	2.15	106.83	102.48
2	A	501	UDX	C5'-C4'-C3'	-2.12	107.06	109.67
2	B	502	UDX	O3A-PB-O3B	2.12	106.76	102.48
2	F	501	UDX	PA-O3A-PB	2.10	140.02	132.83
2	F	500	UDX	PA-O3A-PB	2.07	139.92	132.83
2	C	501	UDX	O3A-PB-O3B	2.05	106.62	102.48
2	C	500	UDX	C5'-O5'-C1'	2.03	116.47	112.38

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	UDX	C1'-O3B-PB-O2B
2	C	500	UDX	O4D-C1D-N1-C6
2	C	500	UDX	C2D-C1D-N1-C6
2	A	501	UDX	C1'-O3B-PB-O2B
2	B	501	UDX	C1'-O3B-PB-O2B
2	B	501	UDX	O4D-C1D-N1-C6
2	B	501	UDX	C2D-C1D-N1-C6

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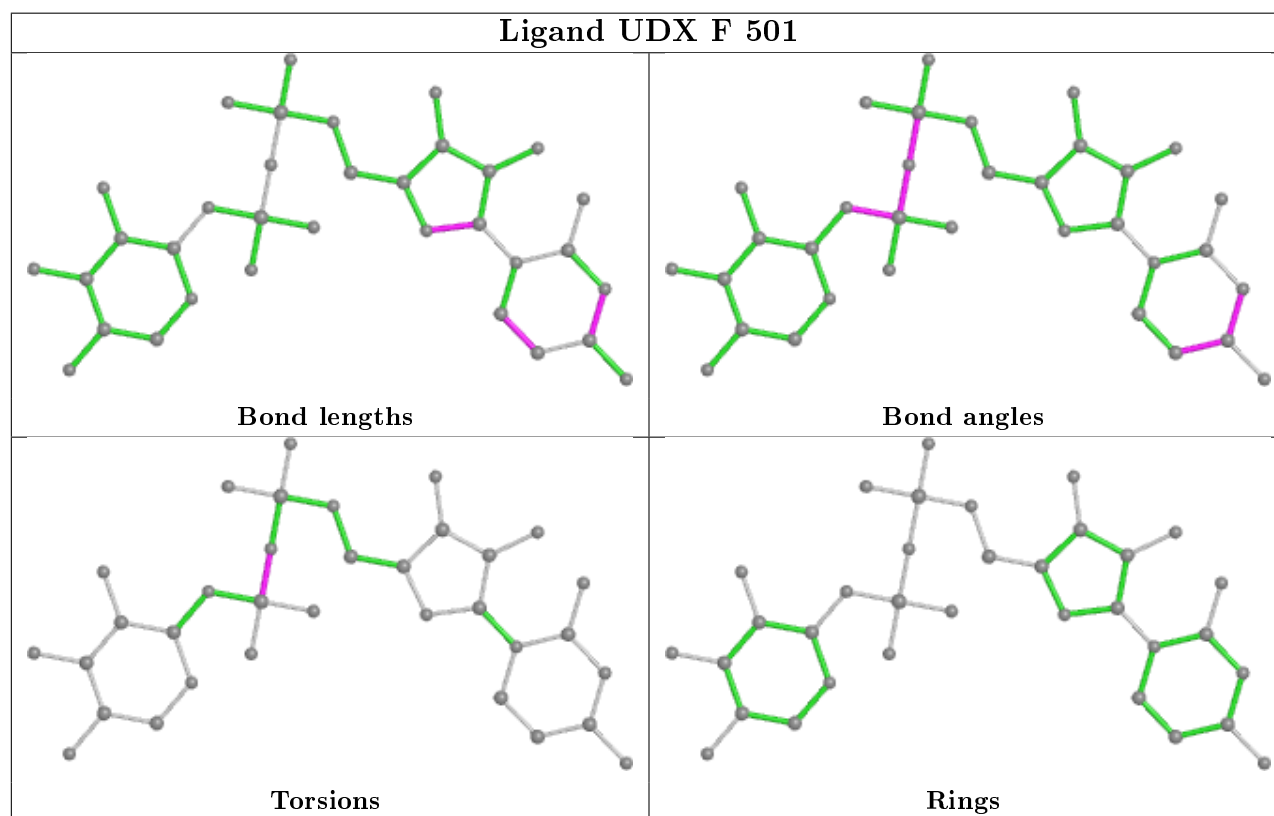
Mol	Chain	Res	Type	Atoms
2	F	500	UDX	C1'-O3B-PB-O2B
2	F	500	UDX	C1'-O3B-PB-O3A
2	A	501	UDX	C2'-C1'-O3B-PB
2	B	501	UDX	C2'-C1'-O3B-PB
2	C	500	UDX	C1'-O3B-PB-O3A
2	B	501	UDX	C1'-O3B-PB-O3A
2	C	500	UDX	C2'-C1'-O3B-PB
2	A	501	UDX	O4D-C4D-C5D-O5D
2	A	501	UDX	C1'-O3B-PB-O3A
2	F	501	UDX	PA-O3A-PB-O3B
2	B	502	UDX	PA-O3A-PB-O3B
2	C	501	UDX	PA-O3A-PB-O3B
2	D	501	UDX	PA-O3A-PB-O3B
2	E	501	UDX	PA-O3A-PB-O3B
2	A	502	UDX	PA-O3A-PB-O3B
2	B	502	UDX	C1'-O3B-PB-O3A
2	C	501	UDX	C1'-O3B-PB-O3A
2	A	502	UDX	C1'-O3B-PB-O3A
2	F	500	UDX	C1'-O3B-PB-O1B
2	E	501	UDX	C1'-O3B-PB-O3A
2	A	501	UDX	C3D-C4D-C5D-O5D
2	B	502	UDX	PB-O3A-PA-O2A
2	F	500	UDX	PA-O3A-PB-O2B
2	A	502	UDX	PB-O3A-PA-O2A
2	B	501	UDX	O4D-C4D-C5D-O5D
2	F	500	UDX	O4D-C4D-C5D-O5D
2	C	500	UDX	O4D-C4D-C5D-O5D
2	D	501	UDX	C1'-O3B-PB-O3A
2	F	501	UDX	PA-O3A-PB-O1B
2	B	502	UDX	PB-O3A-PA-O1A
2	C	501	UDX	PB-O3A-PA-O1A
2	C	501	UDX	PB-O3A-PA-O2A
2	A	501	UDX	C1'-O3B-PB-O1B
2	D	501	UDX	PB-O3A-PA-O1A
2	D	501	UDX	PB-O3A-PA-O2A
2	E	501	UDX	PA-O3A-PB-O2B
2	E	501	UDX	PB-O3A-PA-O2A
2	F	500	UDX	PA-O3A-PB-O1B
2	A	502	UDX	PA-O3A-PB-O2B

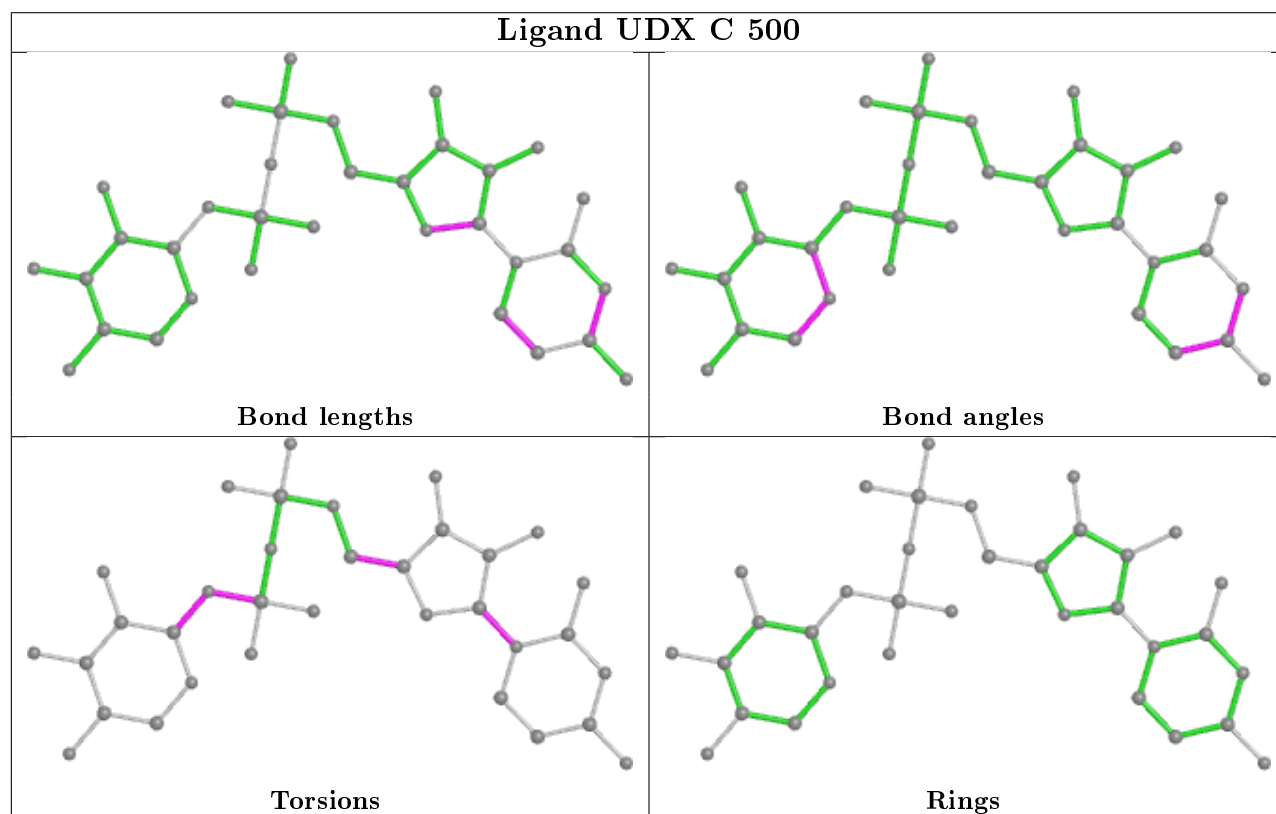
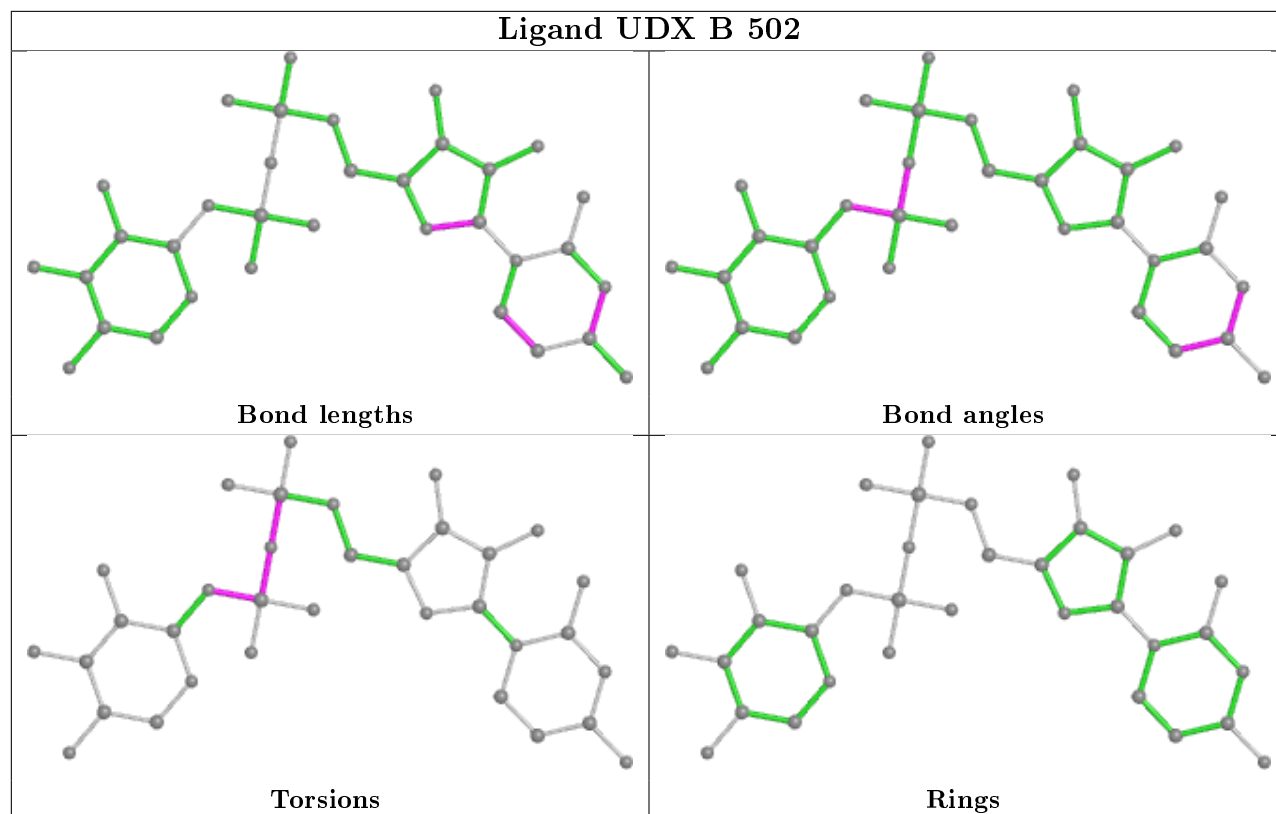
There are no ring outliers.

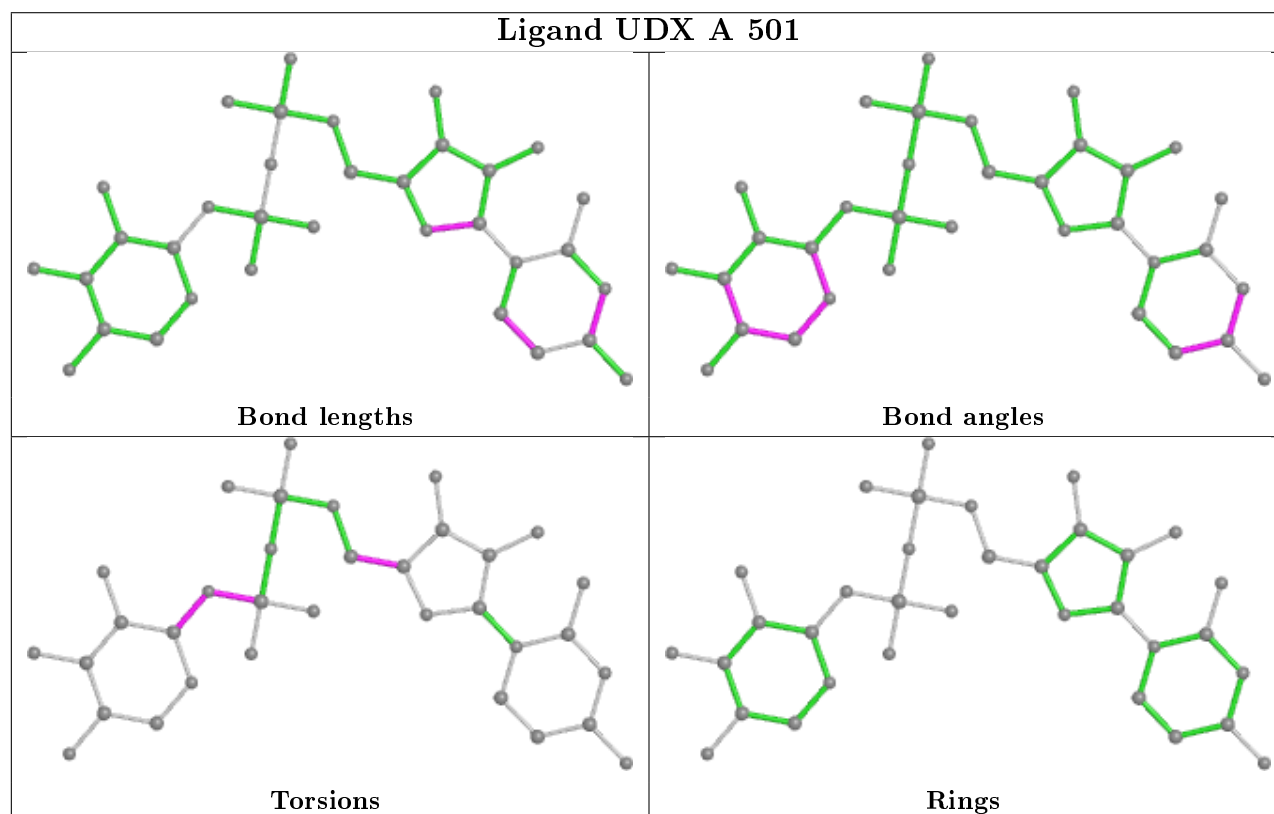
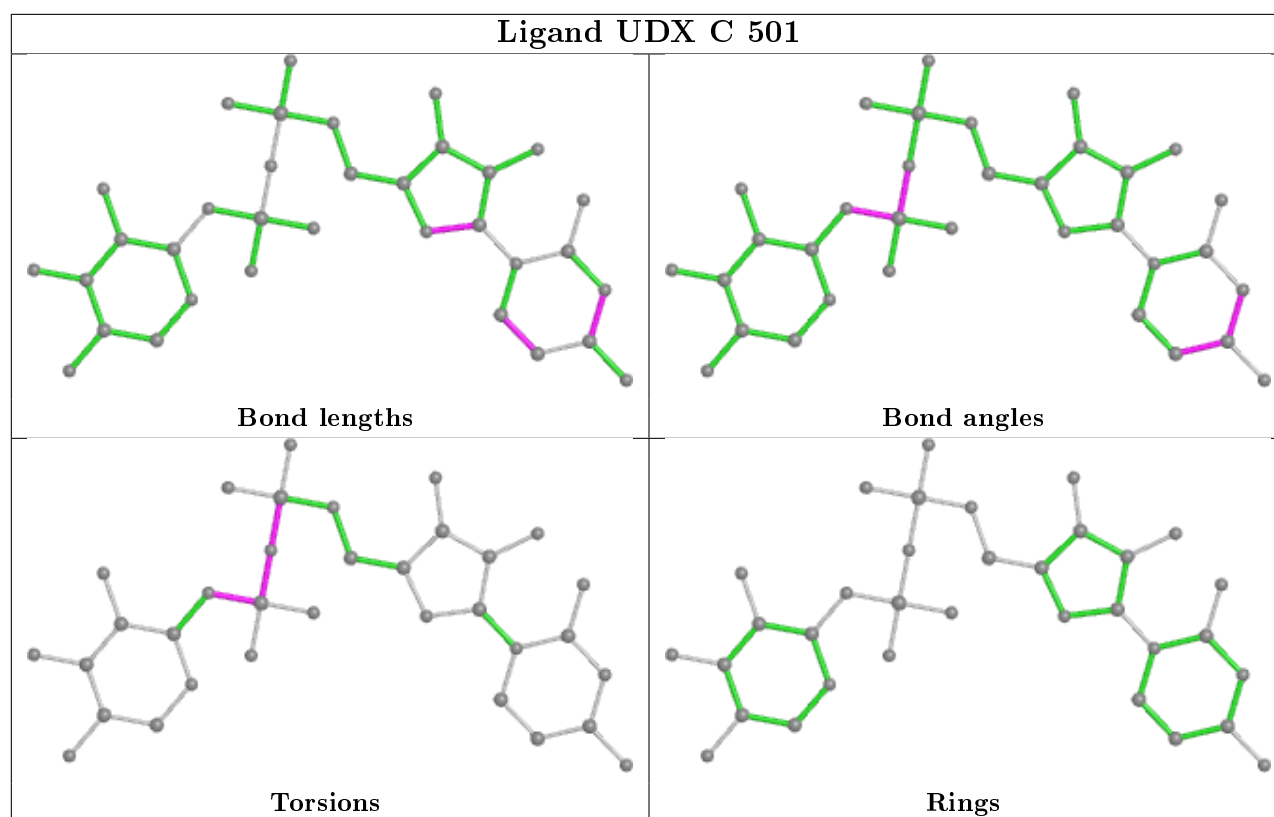
1 monomer is involved in 1 short contact:

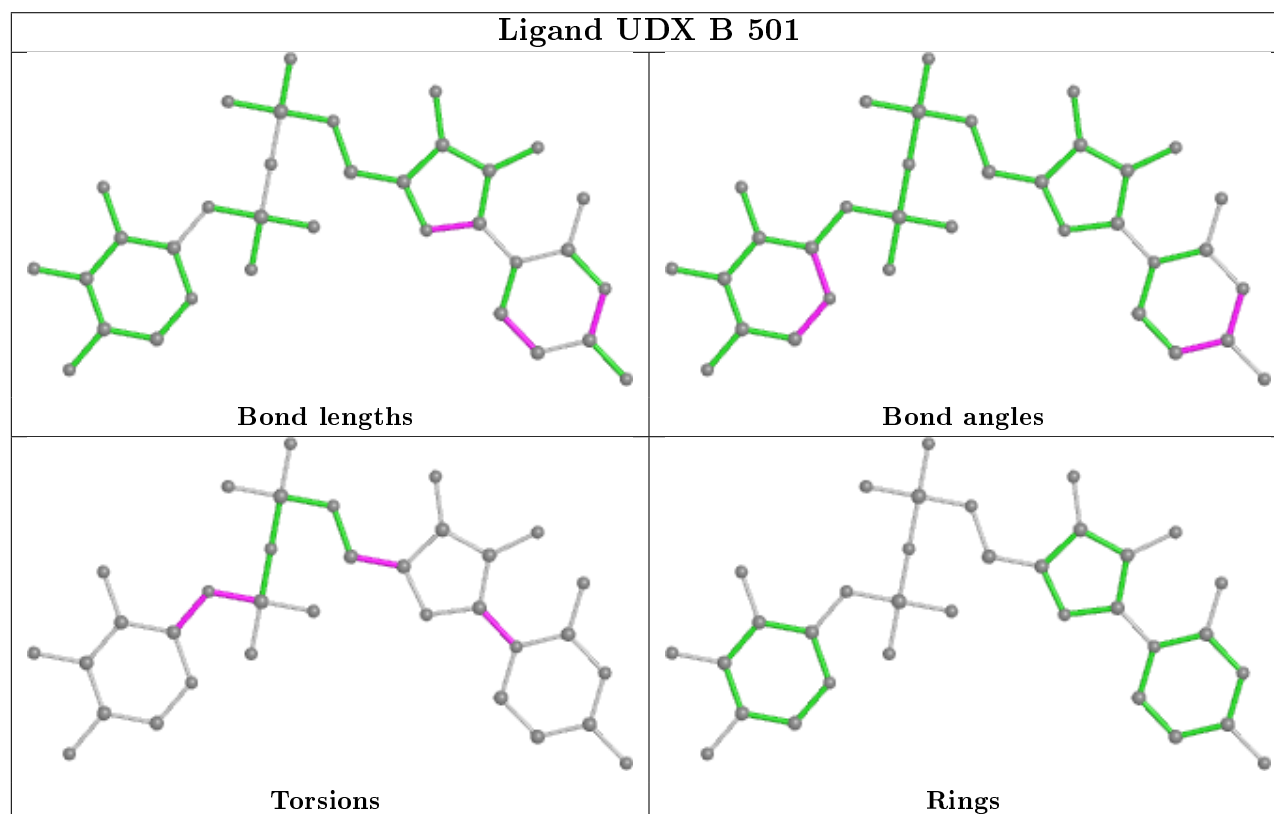
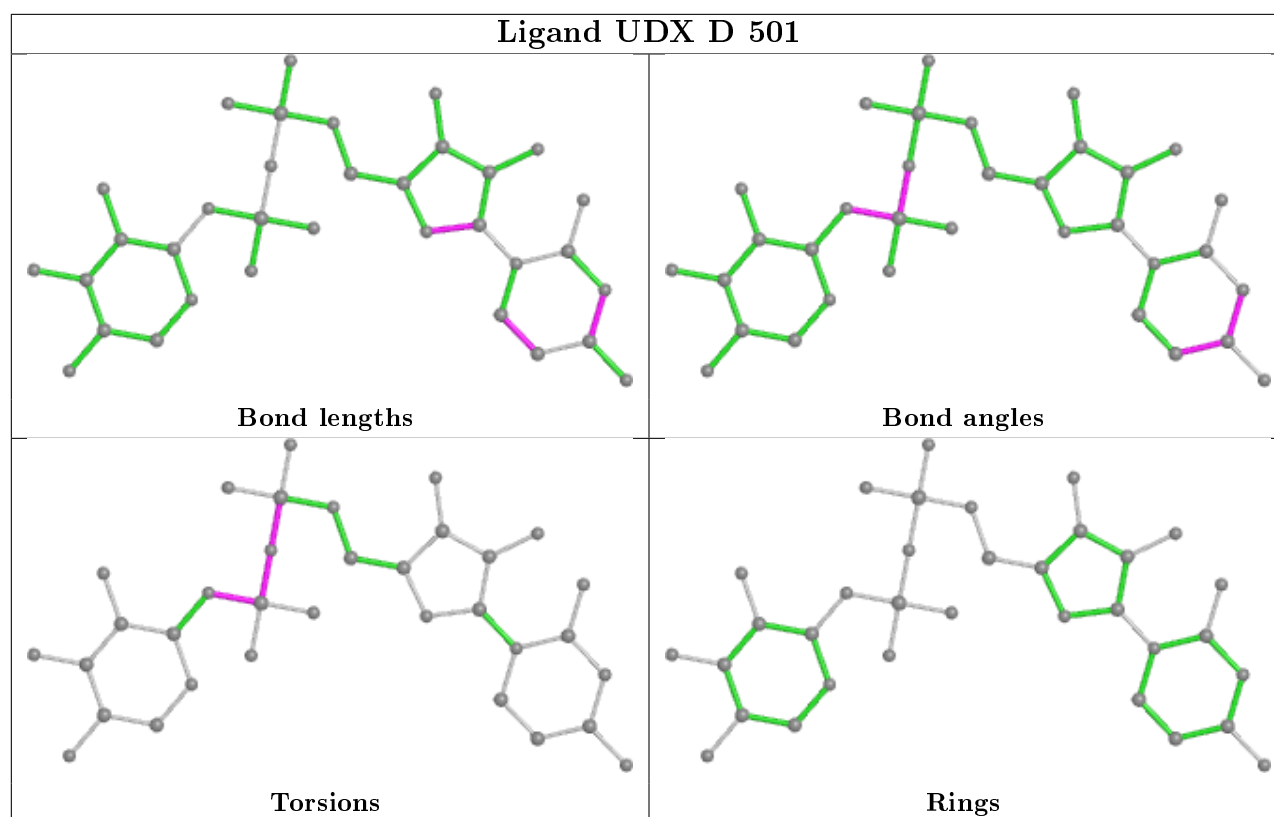
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	UDX	1	0

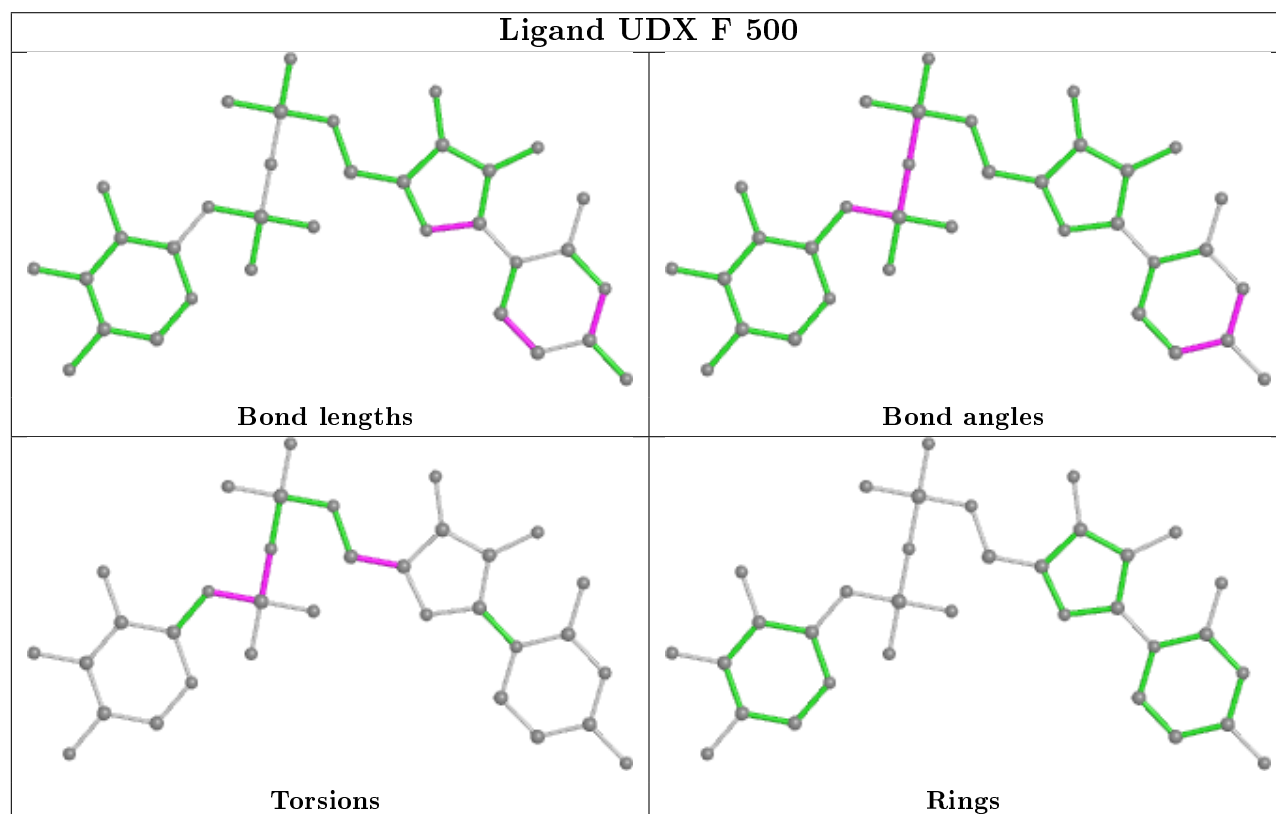
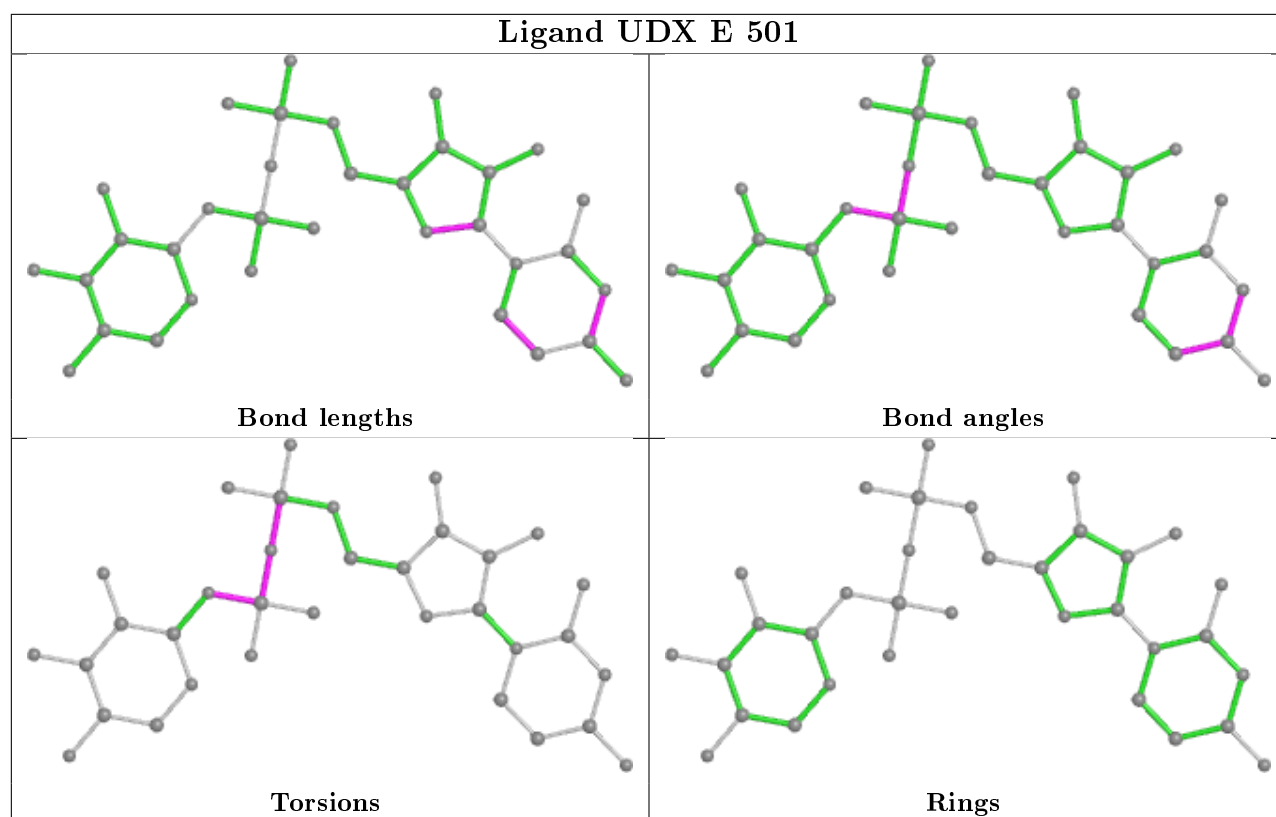
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

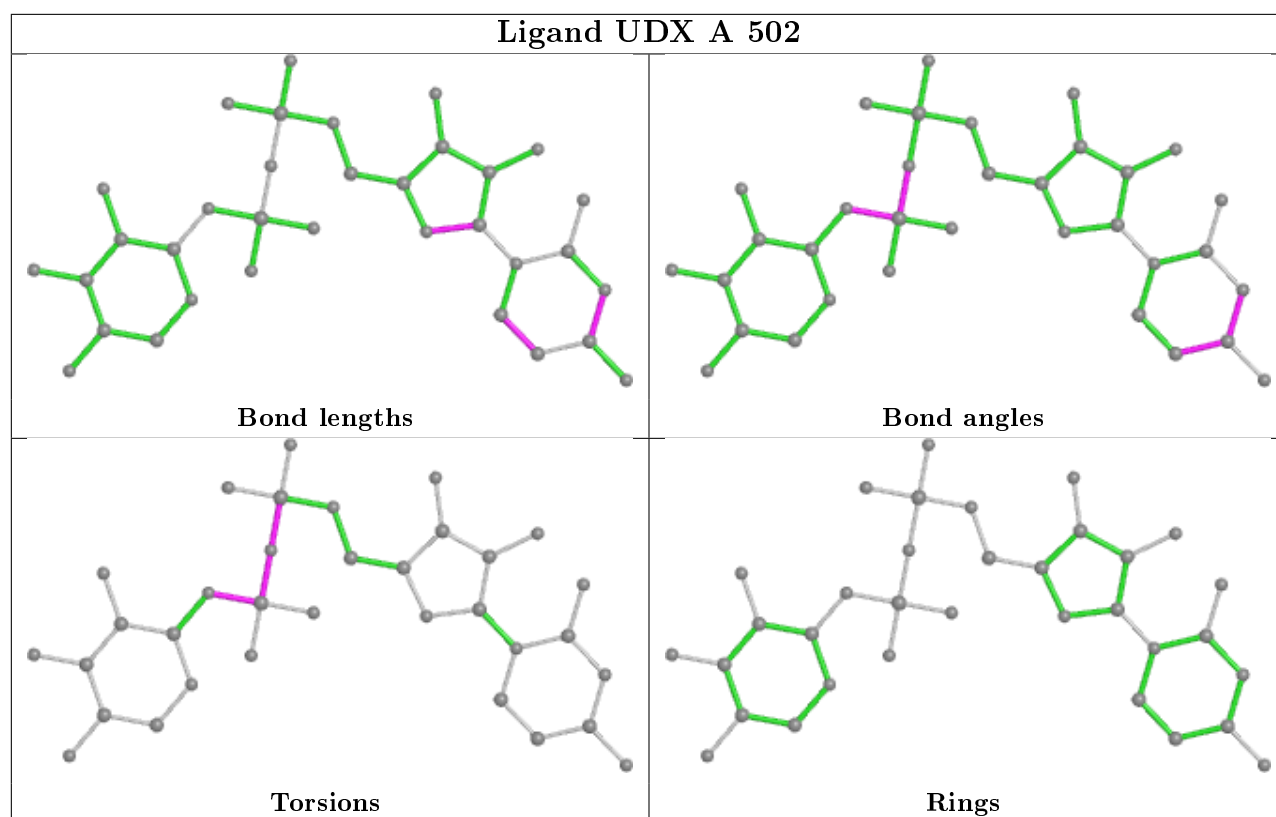












5.7 Other polymers [i](#)

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

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	461/494 (93%)	-0.08	5 (1%) 80 79	22, 33, 52, 115	0
1	B	459/494 (92%)	0.08	4 (0%) 84 83	22, 40, 62, 124	0
1	C	461/494 (93%)	0.14	7 (1%) 73 72	23, 38, 69, 108	0
1	D	449/494 (90%)	0.24	16 (3%) 42 41	24, 46, 81, 107	0
1	E	447/494 (90%)	0.04	8 (1%) 68 66	22, 34, 60, 104	0
1	F	459/494 (92%)	0.50	27 (5%) 22 21	26, 54, 83, 130	0
All	All	2736/2964 (92%)	0.15	67 (2%) 59 56	22, 40, 74, 130	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	151	ASN	5.4
1	C	387	GLU	4.6
1	D	2	PHE	4.4
1	B	382	HIS	4.3
1	D	286	TYR	4.1
1	D	152	LEU	4.1
1	F	151	ASN	3.9
1	E	286	TYR	3.9
1	F	328	ASP	3.8
1	F	323	PHE	3.7
1	D	90	ASN	3.6
1	A	388	ASP	3.5
1	F	431	LYS	3.5
1	E	104	ALA	3.5
1	B	383	PRO	3.4
1	E	150	PRO	3.4
1	A	389	ASP	3.3
1	F	190	ARG	3.3
1	F	326	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	148	THR	3.2
1	E	105	ASP	3.1
1	C	437	PHE	3.0
1	A	382	HIS	3.0
1	E	148	THR	3.0
1	E	90	ASN	2.9
1	F	2	PHE	2.8
1	D	385	VAL	2.8
1	F	63	SER	2.7
1	F	122	GLY	2.7
1	F	320	ASP	2.7
1	F	382	HIS	2.7
1	D	108	TYR	2.7
1	D	123	TYR	2.7
1	E	383	PRO	2.7
1	F	450	ASN	2.7
1	D	142	ARG	2.6
1	F	361	GLY	2.6
1	D	153	ASN	2.6
1	F	426	GLU	2.6
1	E	106	LEU	2.5
1	B	392	SER	2.5
1	F	399	LYS	2.5
1	F	30	ILE	2.4
1	D	105	ASP	2.4
1	F	459	ILE	2.4
1	D	149	LYS	2.4
1	C	382	HIS	2.4
1	F	325	THR	2.4
1	D	121	ASN	2.4
1	F	438	ILE	2.4
1	C	363	HIS	2.3
1	F	422	GLU	2.2
1	D	147	ASN	2.2
1	A	255	ILE	2.2
1	D	150	PRO	2.2
1	F	391	VAL	2.2
1	B	447	GLY	2.2
1	F	408	ALA	2.2
1	F	456	GLY	2.2
1	F	123	TYR	2.1
1	F	432	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	389	ASP	2.1
1	F	454	THR	2.1
1	F	406	ASP	2.1
1	C	383	PRO	2.1
1	A	383	PRO	2.0
1	C	356	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

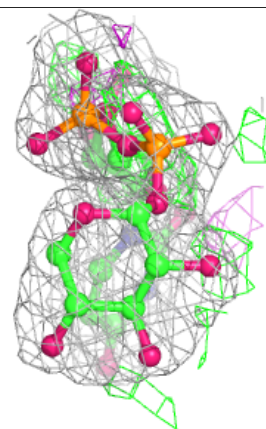
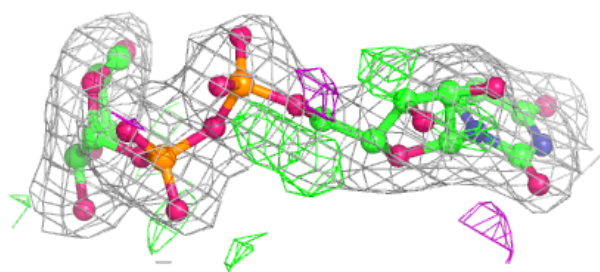
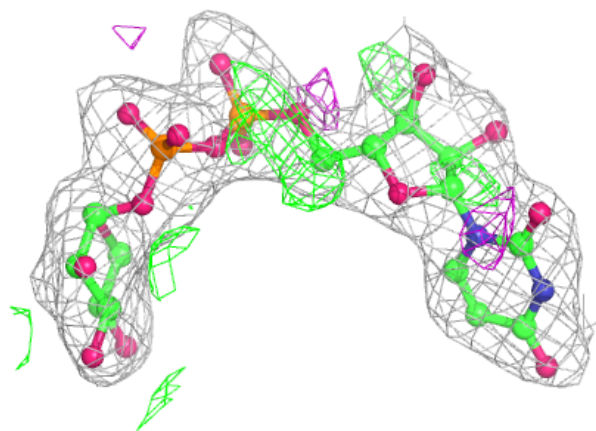
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	D	502	1/1	0.81	0.12	70,70,70,70	0
3	CL	B	503	1/1	0.87	0.11	75,75,75,75	0
3	CL	A	503	1/1	0.94	0.07	56,56,56,56	0
2	UDX	F	500	34/34	0.94	0.16	33,49,57,61	0
2	UDX	B	502	34/34	0.96	0.14	20,28,34,36	0
2	UDX	F	501	34/34	0.96	0.15	28,35,42,53	0
2	UDX	A	501	34/34	0.97	0.11	23,29,35,40	0
2	UDX	D	501	34/34	0.97	0.12	22,31,36,39	0
2	UDX	C	500	34/34	0.97	0.14	23,33,44,47	0
2	UDX	B	501	34/34	0.97	0.14	26,36,40,46	0
2	UDX	C	501	34/34	0.97	0.14	24,29,33,35	0
2	UDX	A	502	34/34	0.97	0.13	9,27,34,36	0
2	UDX	E	501	34/34	0.98	0.14	18,27,30,34	0

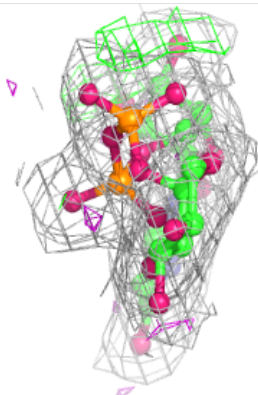
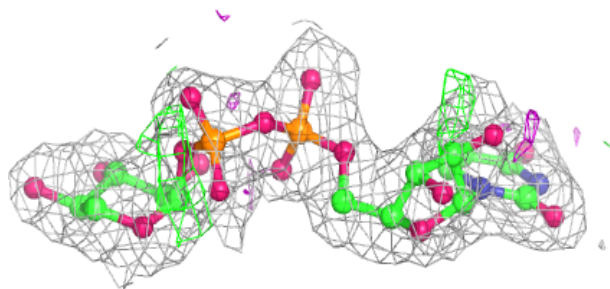
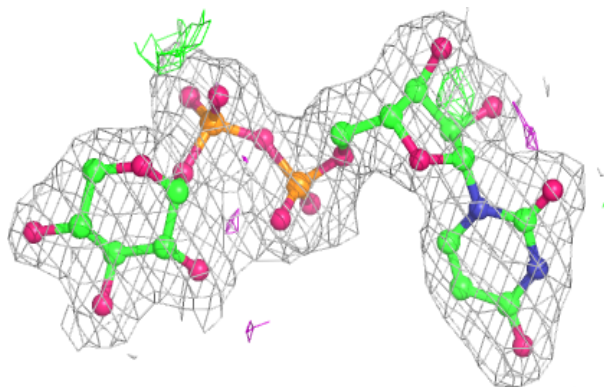
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around UDX 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)

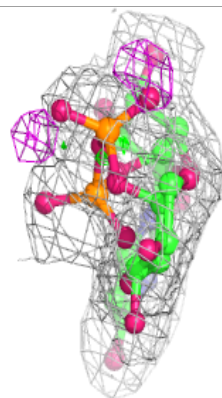
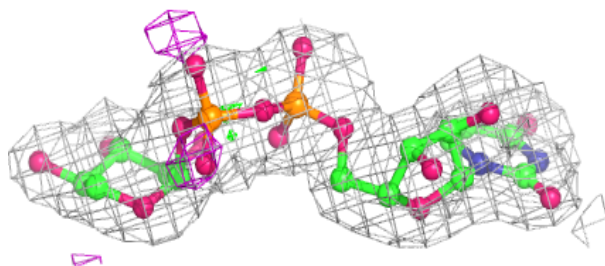
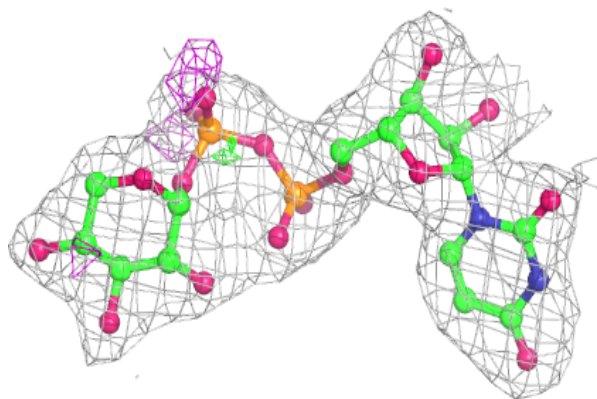
**Electron density around UDX B 502:**

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

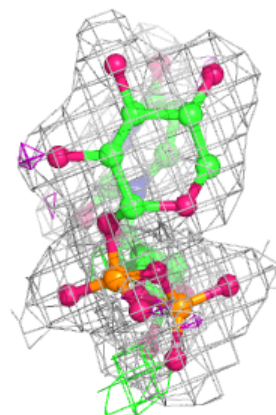
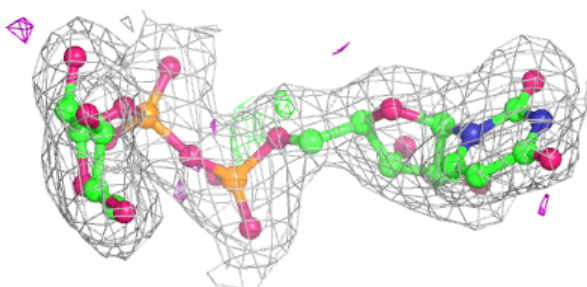
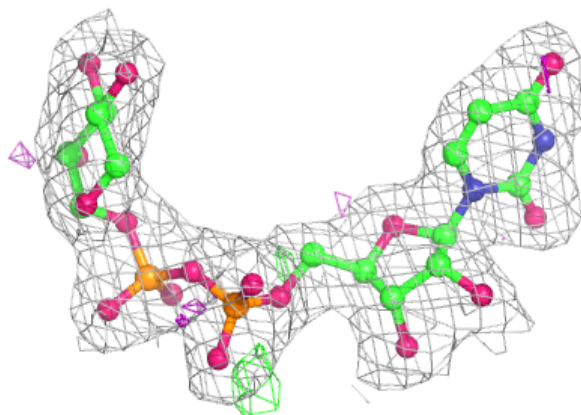


Electron density around UDX F 501:

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

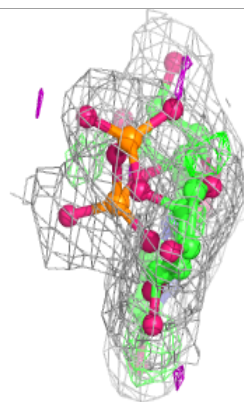
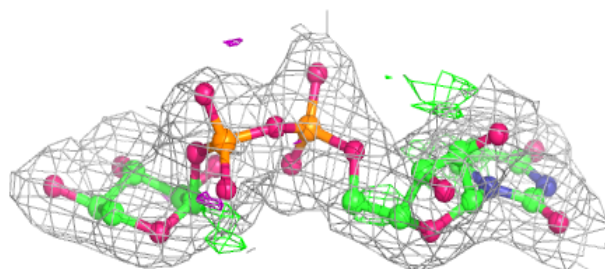
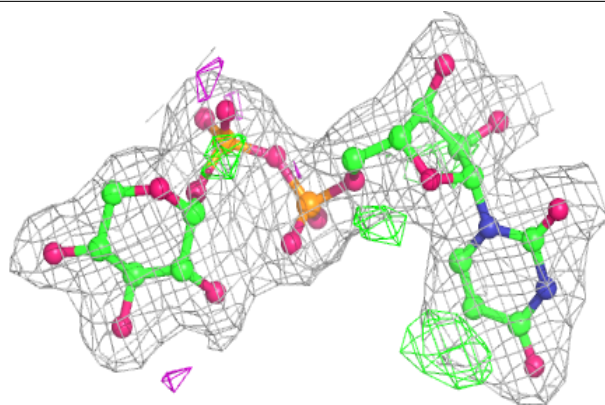
**Electron density around UDX A 501:**

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

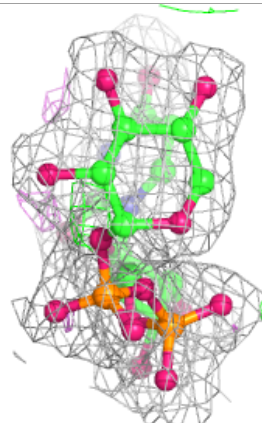
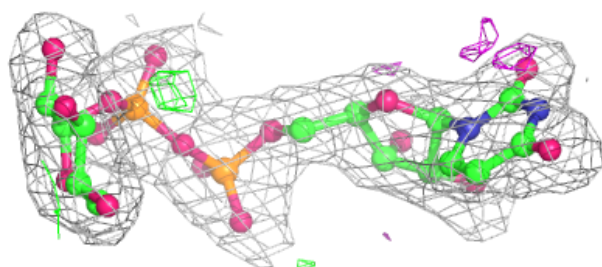
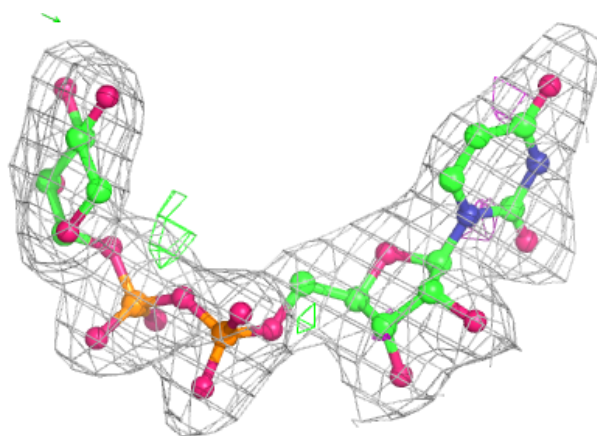


Electron density around UDX D 501:

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

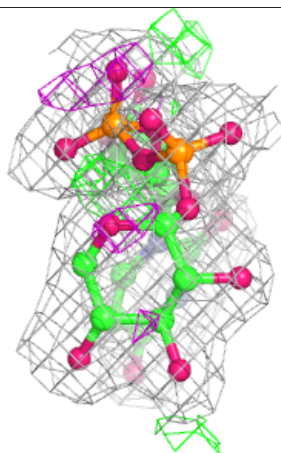
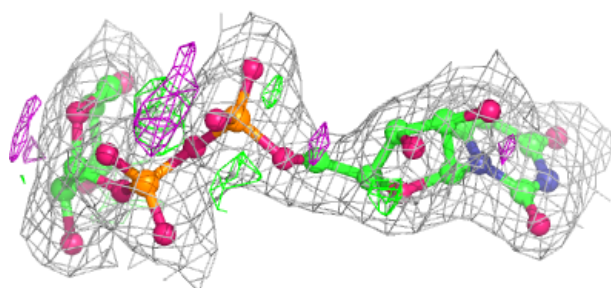
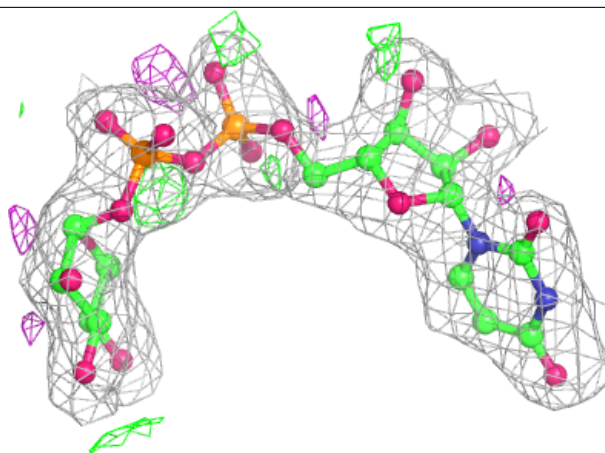
**Electron density around UDX C 500:**

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

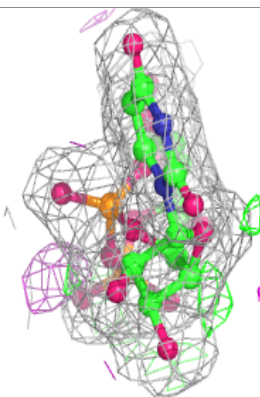
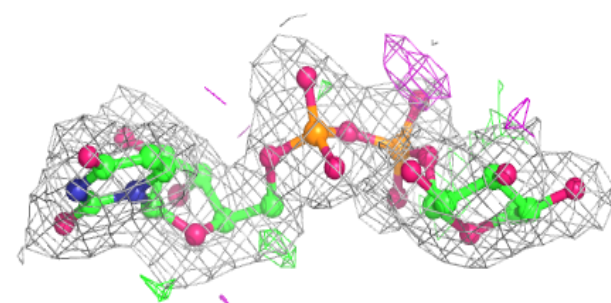
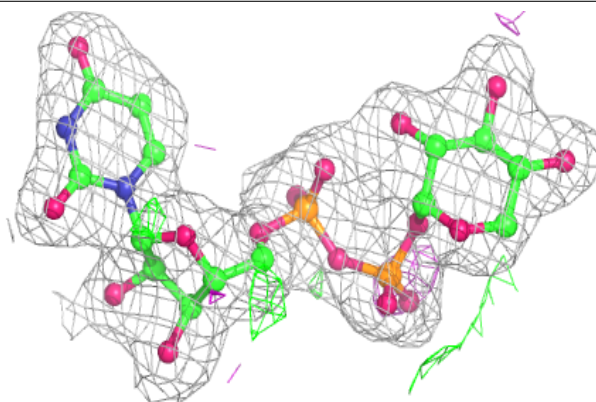


Electron density around UDX B 501:

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

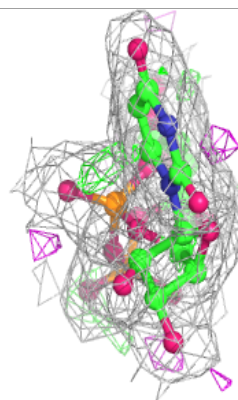
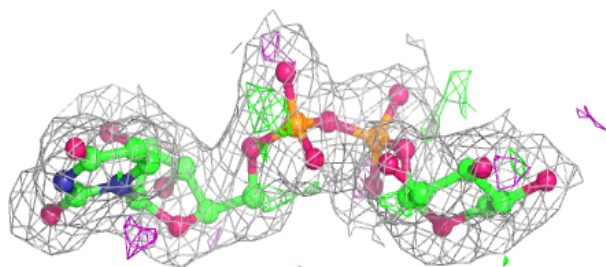
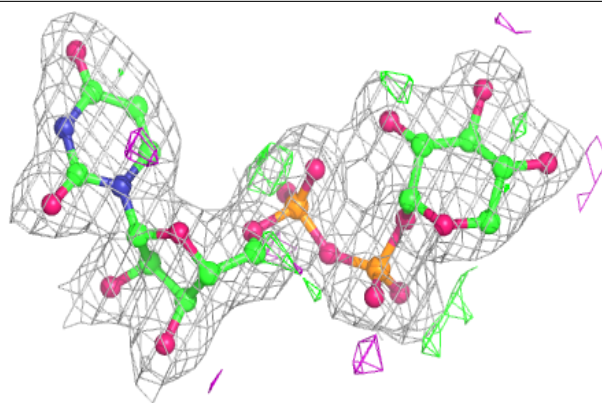
**Electron density around UDX C 501:**

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

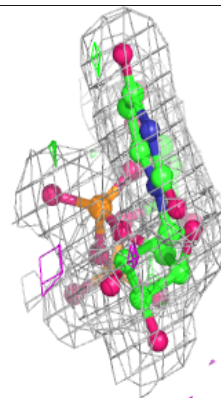
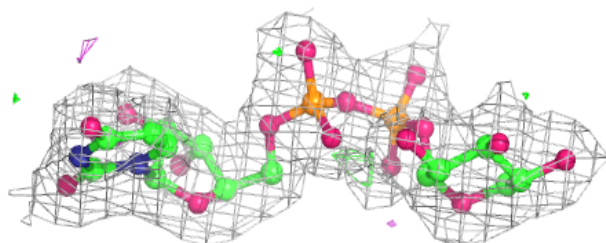
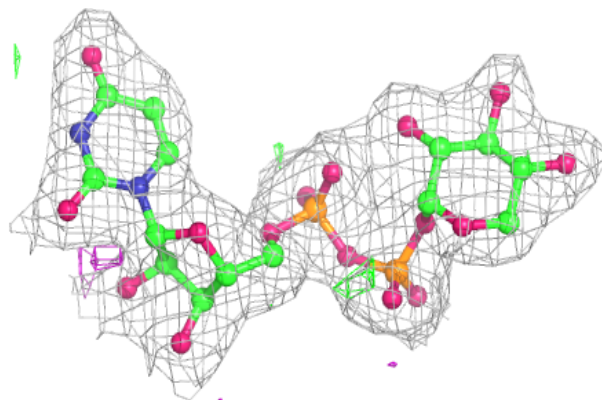


Electron density around UDX A 502:

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

**Electron density around UDX 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)



6.5 Other polymers

There are no such residues in this entry.