



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:11 PM UTC

PDB ID : 6OM8 / pdb_00006om8
Title : Caenorhabditis Elegans UDP-Glucose Dehydrogenase in complex with UDP-Xylose
Authors : Beattie, N.R.; McDonald, W.E.; Hicks Sirmans, T.N.; Wood, Z.A.
Deposited on : 2019-04-18
Resolution : 2.45 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

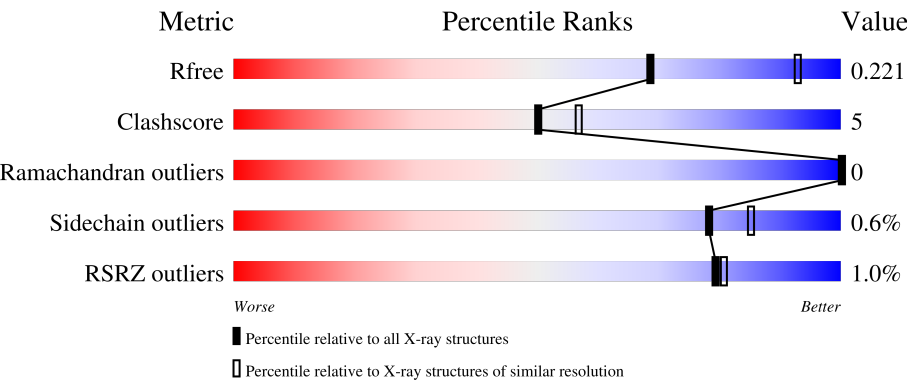
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	481	84%11% . .
1	B	481	2% 84%12% .
1	C	481	% 86%9% . .
1	D	481	% 83%14% .
1	E	481	% 86%10% .

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Mol	Chain	Length	Quality of chain
1	F	481	85%11%.
1	G	481	84%12%.
1	H	481	86%10%.
1	I	481	% 84%12%.
1	J	481	2% 81%12%. 5%
1	K	481	% 85%11%.
1	L	481	% 85%10%..

2 Entry composition

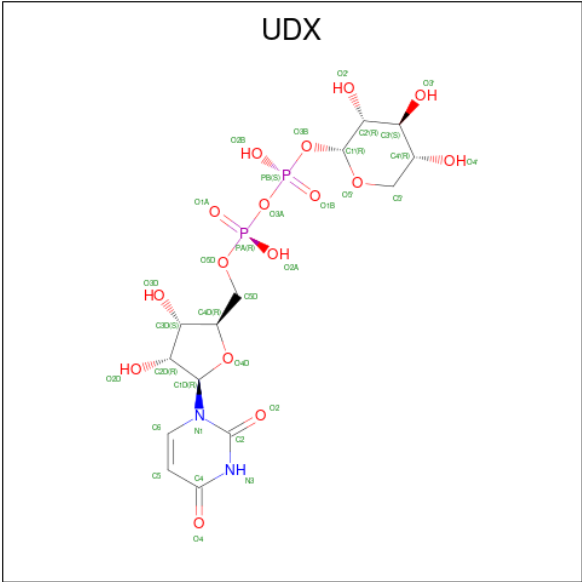
There are 3 unique types of molecules in this entry. The entry contains 44931 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	463	Total	C	N	O	S	0	0	0
			3574	2268	614	677	15			
1	B	463	Total	C	N	O	S	0	1	0
			3577	2270	614	678	15			
1	C	463	Total	C	N	O	S	0	1	0
			3577	2270	614	678	15			
1	D	468	Total	C	N	O	S	0	1	0
			3615	2295	620	685	15			
1	E	461	Total	C	N	O	S	0	2	0
			3564	2261	612	676	15			
1	F	465	Total	C	N	O	S	0	3	0
			3598	2284	617	682	15			
1	G	462	Total	C	N	O	S	0	2	0
			3572	2268	613	676	15			
1	H	462	Total	C	N	O	S	0	3	0
			3580	2275	614	676	15			
1	I	462	Total	C	N	O	S	0	2	0
			3572	2268	613	676	15			
1	J	456	Total	C	N	O	S	0	1	0
			3525	2240	602	669	14			
1	K	464	Total	C	N	O	S	0	2	0
			3591	2280	616	680	15			
1	L	463	Total	C	N	O	S	0	2	0
			3576	2270	614	676	16			

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	H	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	I	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	I	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	J	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	J	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	K	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	K	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	L	1	Total	C	N	O	P	0	0
			34	14	2	16	2		
2	L	1	Total	C	N	O	P	0	0
			34	14	2	16	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		
3	B	90	Total	O	0	0
			90	90		
3	C	125	Total	O	0	0
			125	125		
3	D	135	Total	O	0	0
			135	135		
3	E	117	Total	O	0	0
			117	117		
3	F	123	Total	O	0	0
			123	123		
3	G	74	Total	O	0	0
			74	74		
3	H	107	Total	O	0	0
			107	107		
3	I	74	Total	O	0	0
			74	74		

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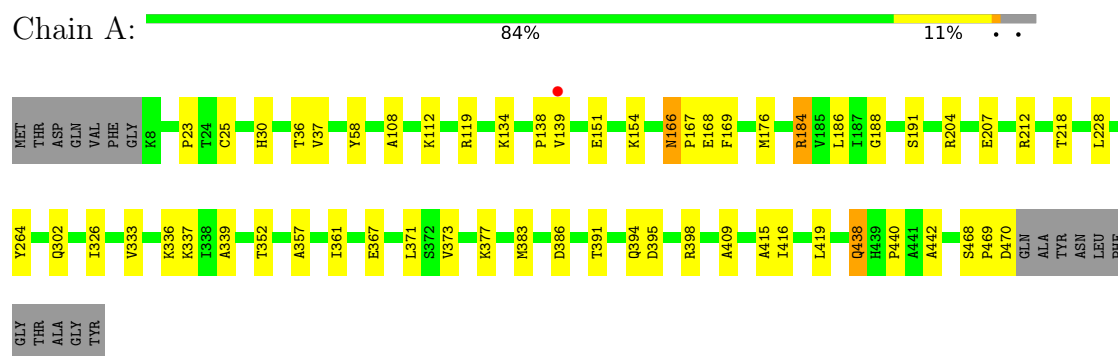
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	42	Total 42	O 42	0	0
3	K	107	Total 107	O 107	0	0
3	L	73	Total 73	O 73	0	0

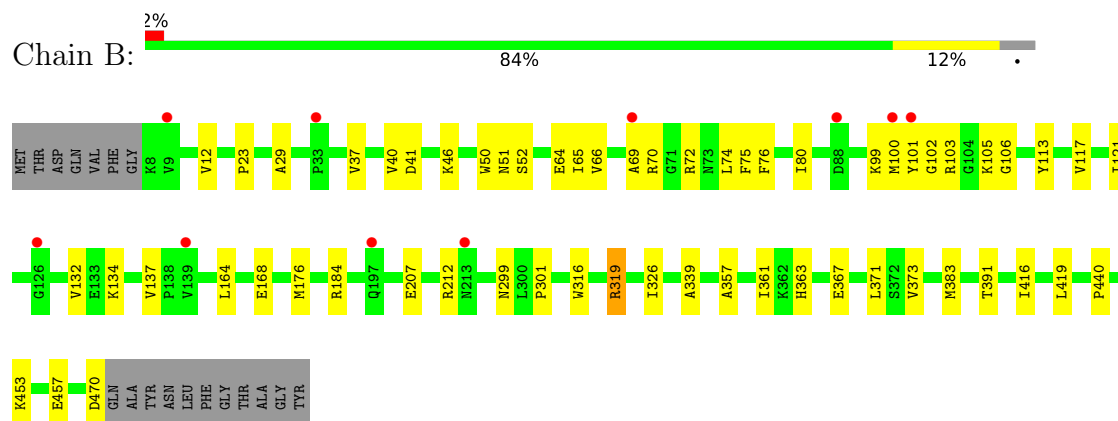
3 Residue-property plots [i](#)

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.

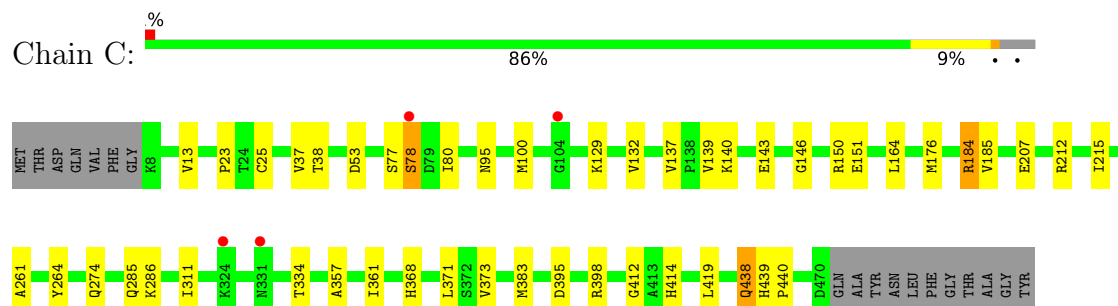
• Molecule 1: UDP-glucose 6-dehydrogenase



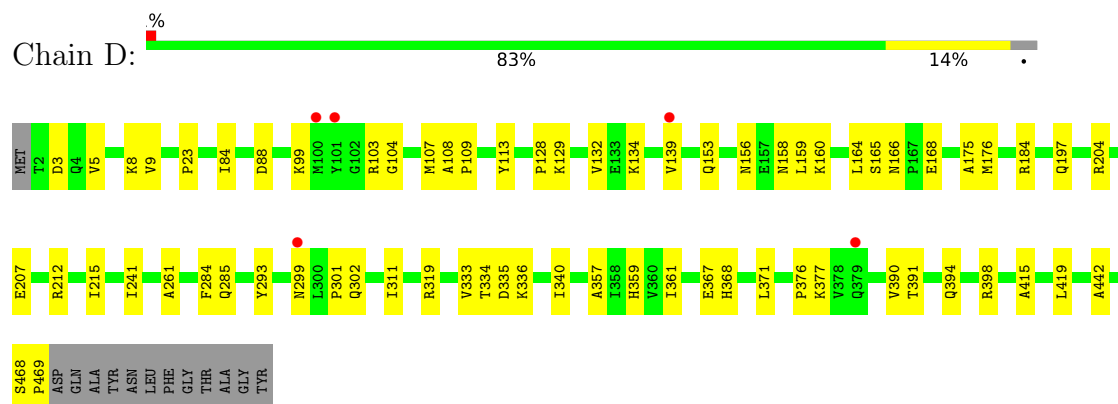
• Molecule 1: UDP-glucose 6-dehydrogenase



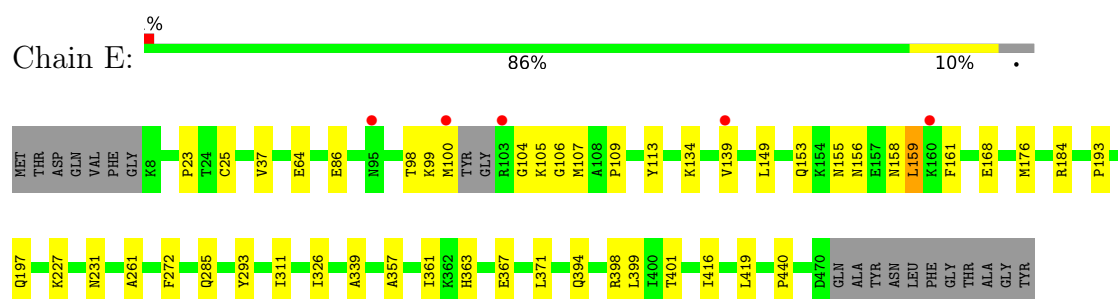
• Molecule 1: UDP-glucose 6-dehydrogenase



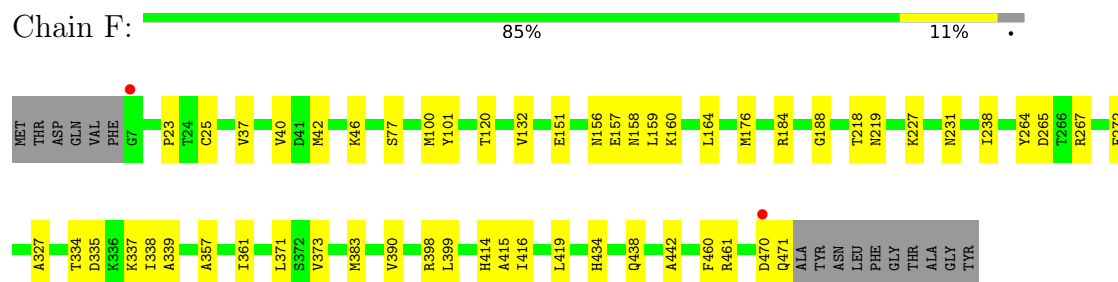
● Molecule 1: UDP-glucose 6-dehydrogenase



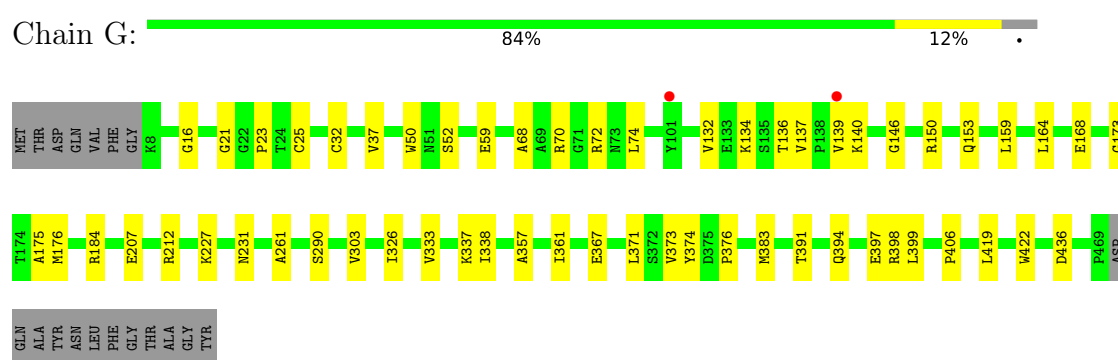
● Molecule 1: UDP-glucose 6-dehydrogenase



● Molecule 1: UDP-glucose 6-dehydrogenase

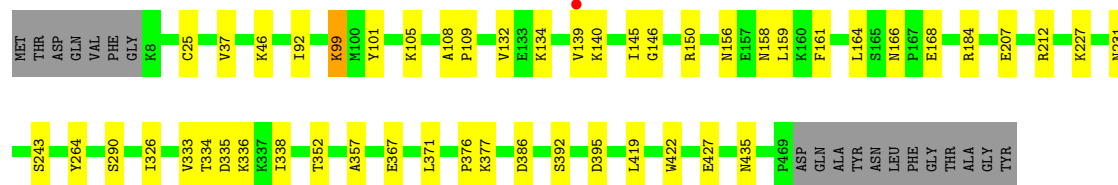


● Molecule 1: UDP-glucose 6-dehydrogenase



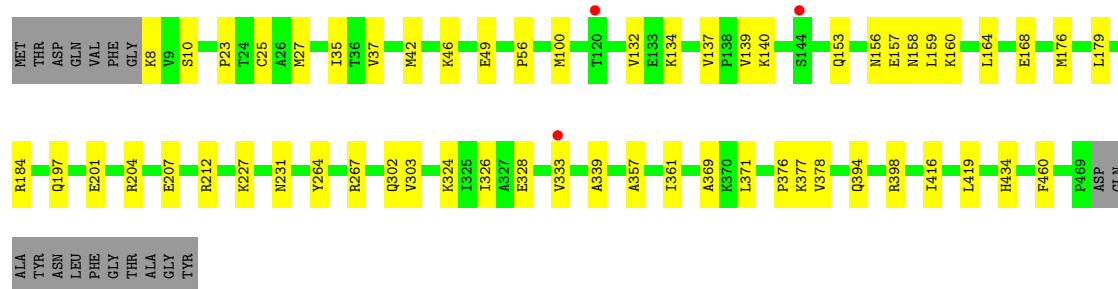
● Molecule 1: UDP-glucose 6-dehydrogenase

Chain H:  86% 10% .



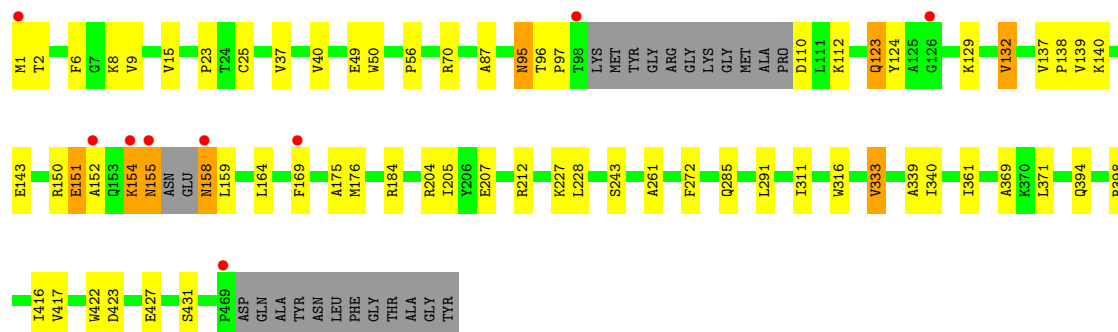
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain I:  84% 12% .



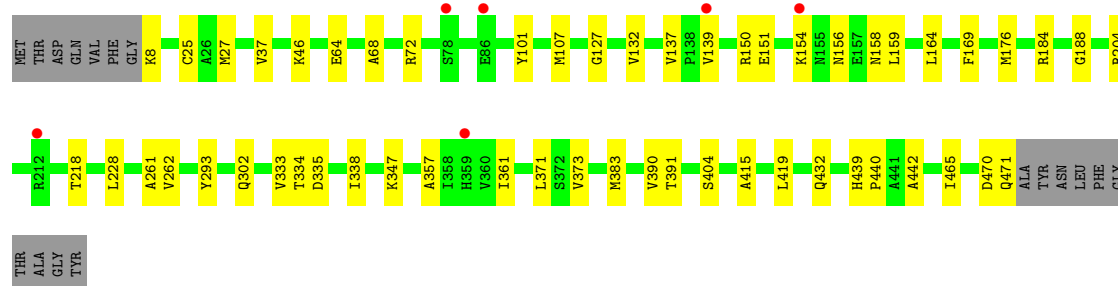
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain J:  81% 12% 5% .

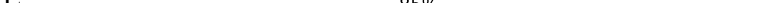


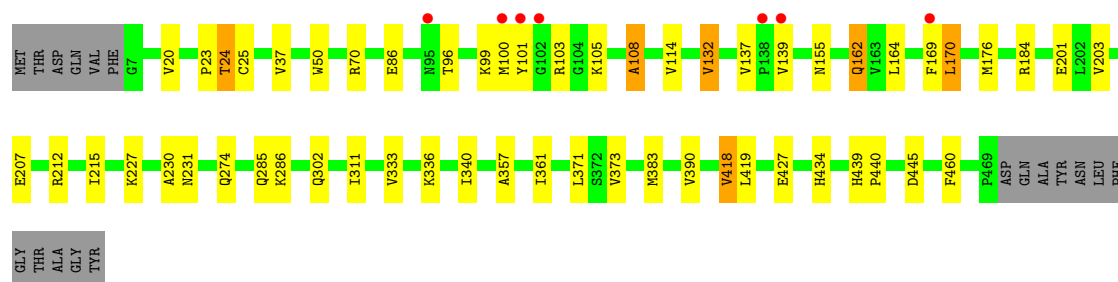
• Molecule 1: UDP-glucose 6-dehydrogenase

Chain K:  85% 11% .



- Molecule 1: UDP-glucose 6-dehydrogenase

Chain L:  85% 10% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	157.71Å 168.17Å 279.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.70 – 2.45 52.70 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.1 (52.70-2.45) 98.1 (52.70-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.194 , 0.220 0.194 , 0.221	Depositor DCC
R_{free} test set	1847 reflections (0.64%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	44931	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% 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: 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	0.59	1/3643 (0.0%)	0.53	5/4941 (0.1%)
1	B	0.51	1/3649 (0.0%)	0.53	2/4949 (0.0%)
1	C	0.51	1/3649 (0.0%)	0.54	2/4949 (0.0%)
1	D	0.53	2/3688 (0.1%)	0.50	3/5002 (0.1%)
1	E	0.48	0/3637	0.51	2/4931 (0.0%)
1	F	0.56	1/3676 (0.0%)	0.51	1/4985 (0.0%)
1	G	0.40	0/3647	0.47	1/4946 (0.0%)
1	H	0.52	0/3658	0.48	3/4961 (0.1%)
1	I	0.40	0/3647	0.44	0/4946
1	J	0.57	0/3594	0.63	9/4875 (0.2%)
1	K	0.50	0/3666	0.54	3/4972 (0.1%)
1	L	0.50	0/3651	0.50	4/4951 (0.1%)
All	All	0.51	6/43805 (0.0%)	0.52	35/59408 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	338	ILE	C-O	-5.51	1.18	1.24
1	B	319	ARG	C-O	-5.21	1.18	1.24
1	D	165	SER	C-O	-5.19	1.18	1.24
1	D	166	ASN	C-O	-5.11	1.18	1.24
1	A	112	LYS	C-O	-5.07	1.18	1.24
1	C	185	VAL	C-O	-5.01	1.18	1.24

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	427	GLU	N-CA-C	7.91	122.97	113.16
1	J	423	ASP	N-CA-C	7.87	120.75	111.71
1	K	465	ILE	O-C-N	-7.11	115.42	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	123	GLN	N-CA-C	6.80	118.78	111.36
1	A	112	LYS	N-CA-C	6.69	119.42	111.33
1	B	65	ILE	N-CA-C	6.67	117.46	110.72
1	L	390	VAL	CB-CA-C	6.49	119.01	111.55
1	J	132	VAL	N-CA-C	6.12	116.68	108.11
1	C	438	GLN	N-CA-C	-6.09	102.67	110.53
1	G	391	THR	N-CA-C	6.06	118.47	108.48
1	H	99	LYS	N-CA-C	-5.97	101.57	110.23
1	B	391	THR	N-CA-C	5.92	118.25	108.48
1	J	422	TRP	O-C-N	-5.84	115.84	122.97
1	H	99	LYS	CB-CA-C	5.82	119.38	109.72
1	J	151	GLU	N-CA-C	-5.76	104.92	111.14
1	K	390	VAL	CB-CA-C	5.64	118.04	111.55
1	J	96	THR	CA-C-N	-5.63	114.80	120.21
1	J	96	THR	C-N-CA	-5.63	114.80	120.21
1	C	80	ILE	CB-CA-C	-5.62	108.36	113.70
1	L	108	ALA	CA-C-N	-5.49	114.32	120.14
1	L	108	ALA	C-N-CA	-5.49	114.32	120.14
1	E	159	LEU	N-CA-C	5.46	117.20	108.41
1	L	203	VAL	N-CA-C	-5.43	105.24	110.72
1	J	6	PHE	N-CA-C	5.42	118.35	111.69
1	A	166	ASN	CA-C-N	-5.37	114.43	119.85
1	A	166	ASN	C-N-CA	-5.37	114.43	119.85
1	F	390	VAL	CB-CA-C	5.37	120.09	111.29
1	D	390	VAL	CB-CA-C	5.35	117.71	111.55
1	A	391	THR	N-CA-C	5.32	117.25	108.48
1	H	377	LYS	N-CA-C	5.31	121.16	114.31
1	K	391	THR	N-CA-C	5.28	122.05	110.80
1	A	108	ALA	N-CA-C	5.22	117.51	110.31
1	E	104	GLY	N-CA-C	-5.15	106.96	114.90
1	D	391	THR	N-CA-C	5.11	121.68	110.80
1	D	5	VAL	N-CA-C	5.07	115.79	110.62

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	3574	0	3584	38	0
1	B	3577	0	3589	52	0
1	C	3577	0	3589	33	0
1	D	3615	0	3625	44	0
1	E	3564	0	3581	36	0
1	F	3598	0	3616	41	0
1	G	3572	0	3590	42	0
1	H	3580	0	3604	33	0
1	I	3572	0	3590	41	0
1	J	3525	0	3536	63	0
1	K	3591	0	3608	34	0
1	L	3576	0	3593	42	0
2	A	68	0	40	0	0
2	B	68	0	40	0	0
2	C	68	0	40	1	0
2	D	68	0	40	2	0
2	E	68	0	40	1	0
2	F	68	0	40	1	0
2	G	68	0	40	1	0
2	H	68	0	40	0	0
2	I	68	0	40	1	0
2	J	68	0	40	1	0
2	K	68	0	40	0	0
2	L	68	0	40	0	0
3	A	127	0	0	5	0
3	B	90	0	0	4	0
3	C	125	0	0	4	0
3	D	135	0	0	3	0
3	E	117	0	0	6	0
3	F	123	0	0	3	0
3	G	74	0	0	5	0
3	H	107	0	0	1	0
3	I	74	0	0	4	0
3	J	42	0	0	1	0
3	K	107	0	0	4	0
3	L	73	0	0	4	0
All	All	44931	0	43585	464	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 5.

All (464) 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:E:184:ARG:NH1	1:F:265:ASP:HB2	1.49	1.27
1:B:40:VAL:HG11	1:B:80:ILE:HG12	1.31	1.12
1:A:204:ARG:HD3	3:A:663:HOH:O	1.53	1.07
1:I:333:VAL:HG12	1:I:369:ALA:HB2	1.36	1.07
1:E:184:ARG:HH12	1:F:265:ASP:HB2	0.97	1.06
1:D:109:PRO:HG3	1:D:139:VAL:HG21	1.37	1.05
1:J:169:PHE:CE2	1:J:184:ARG:HG3	1.93	1.02
1:J:169:PHE:HE2	1:J:184:ARG:HG3	1.26	1.01
1:E:184:ARG:HH12	1:F:265:ASP:CB	1.74	0.98
1:B:40:VAL:CG1	1:B:80:ILE:HG12	1.93	0.97
1:E:23:PRO:HB3	1:E:176:MET:HE1	1.46	0.94
1:J:155:ASN:ND2	1:J:155:ASN:O	2.00	0.93
1:J:158:ASN:C	1:J:159:LEU:HD22	1.96	0.91
1:J:8:LYS:HE3	1:J:204:ARG:NH2	1.86	0.90
1:B:440:PRO:HB3	1:F:151:GLU:HG3	1.52	0.89
1:J:23:PRO:HB3	1:J:176:MET:HE1	1.56	0.88
1:E:184:ARG:NH1	1:F:265:ASP:CB	2.35	0.87
1:D:153:GLN:HG3	1:D:159:LEU:O	1.75	0.87
1:I:153:GLN:HG3	1:I:159:LEU:O	1.75	0.84
1:A:394:GLN:HG3	3:A:607:HOH:O	1.76	0.84
1:D:302:GLN:HG3	3:D:654:HOH:O	1.77	0.83
1:J:169:PHE:HD1	1:J:227:LYS:HZ3	1.23	0.83
1:J:25:CYS:HB3	1:J:37:VAL:HG11	1.59	0.83
1:D:23:PRO:HB3	1:D:176:MET:HE1	1.60	0.83
1:I:23:PRO:HB3	1:I:176:MET:HE1	1.59	0.83
1:I:333:VAL:CG1	1:I:369:ALA:HB2	2.10	0.81
1:J:110:ASP:OD2	1:J:112:LYS:HG2	1.80	0.81
1:H:159:LEU:HD12	1:H:159:LEU:O	1.81	0.80
1:A:23:PRO:HB3	1:A:176:MET:HE1	1.63	0.80
1:D:109:PRO:HG3	1:D:139:VAL:CG2	2.12	0.79
1:A:440:PRO:HB3	1:C:151:GLU:HG3	1.64	0.79
1:J:169:PHE:HE1	1:J:227:LYS:HD3	1.48	0.78
1:A:151:GLU:HG3	1:E:440:PRO:HB3	1.65	0.78
1:A:36:THR:HG22	3:A:622:HOH:O	1.85	0.77
1:J:123:GLN:HG2	1:J:124:TYR:CE2	2.20	0.77
1:B:23:PRO:HB3	1:B:176:MET:HE1	1.67	0.76
1:C:23:PRO:HB3	1:C:176:MET:HE1	1.66	0.75
1:I:100:MET:HE2	3:I:628:HOH:O	1.86	0.75
1:B:51:ASN:C	1:B:70:ARG:NH2	2.45	0.74
1:J:169:PHE:CE2	1:J:184:ARG:CG	2.69	0.74
1:F:188:GLY:HA2	1:F:218:THR:O	1.86	0.74
1:E:109:PRO:HG2	1:E:139:VAL:HG21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:23:PRO:HB3	1:L:176:MET:HE1	1.71	0.73
1:B:52:SER:C	1:B:70:ARG:HH22	1.95	0.73
1:F:337:LYS:NZ	3:F:601:HOH:O	2.22	0.72
1:F:156:ASN:OD1	1:F:158:ASN:HB2	1.88	0.72
1:F:327:ALA:HB1	1:J:1:MET:HG3	1.71	0.72
1:K:333:VAL:HG21	1:K:338:ILE:HD11	1.71	0.72
1:K:261:ALA:O	1:L:184:ARG:NH2	2.22	0.71
1:J:110:ASP:OD2	1:J:112:LYS:CG	2.38	0.71
1:J:394:GLN:HE21	1:J:398:ARG:NH2	1.89	0.71
1:L:418:VAL:HG22	1:L:445:ASP:HA	1.71	0.71
1:J:95:ASN:OD1	2:J:500:UDX:H5A1	1.90	0.71
1:B:52:SER:O	1:B:70:ARG:NH2	2.21	0.70
1:E:25:CYS:HB3	1:E:37:VAL:HG11	1.74	0.70
1:H:159:LEU:HD13	1:H:161:PHE:CE2	2.26	0.70
1:L:170:LEU:HD12	1:L:170:LEU:C	2.17	0.70
1:F:23:PRO:HB3	1:F:176:MET:HE1	1.73	0.70
1:G:394:GLN:O	1:G:397:GLU:HG2	1.92	0.70
1:L:99:LYS:HG3	1:L:108:ALA:O	1.92	0.69
1:F:25:CYS:HB3	1:F:37:VAL:HG11	1.74	0.69
1:L:361:ILE:HG23	1:L:371:LEU:HD13	1.74	0.69
1:L:162:GLN:HA	1:L:162:GLN:OE1	1.91	0.69
1:L:170:LEU:HD12	1:L:170:LEU:O	1.92	0.69
1:E:153:GLN:HG3	1:E:159:LEU:O	1.92	0.69
1:B:51:ASN:HA	1:B:70:ARG:HD2	1.74	0.68
1:C:261:ALA:O	1:D:184:ARG:NH1	2.26	0.68
1:H:156:ASN:OD1	1:H:158:ASN:HB2	1.94	0.67
1:A:302:GLN:HG3	1:B:316:TRP:CD1	2.30	0.67
1:E:100:MET:HA	1:E:105:LYS:HB2	1.76	0.67
1:G:394:GLN:HG3	1:G:397:GLU:OE2	1.94	0.67
1:I:132:VAL:HG22	1:I:164:LEU:HB2	1.77	0.67
1:D:156:ASN:OD1	1:D:158:ASN:HB2	1.93	0.67
1:I:25:CYS:HB3	1:I:37:VAL:HG11	1.76	0.67
1:H:132:VAL:HG22	1:H:164:LEU:HB2	1.76	0.66
1:K:432:GLN:HG2	3:K:601:HOH:O	1.95	0.65
1:K:132:VAL:HG22	1:K:164:LEU:HB2	1.78	0.65
1:A:25:CYS:HB3	1:A:37:VAL:HG11	1.79	0.65
1:J:169:PHE:CE1	1:J:227:LYS:HD3	2.30	0.65
1:B:12:VAL:HB	1:B:37:VAL:HG12	1.77	0.65
1:E:394:GLN:HB2	3:E:672:HOH:O	1.97	0.64
1:G:23:PRO:HB3	1:G:176:MET:HE1	1.79	0.64
1:F:157:GLU:O	1:F:160:LYS:HE2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:MET:CE	3:I:628:HOH:O	2.43	0.64
1:G:25:CYS:HB3	1:G:37:VAL:HG11	1.80	0.64
1:K:334:THR:O	1:K:335:ASP:HB3	1.97	0.64
1:L:169:PHE:CE1	1:L:227:LYS:HD3	2.32	0.64
1:J:139:VAL:HG23	1:J:139:VAL:O	1.97	0.64
1:G:137:VAL:HG12	1:G:137:VAL:O	1.98	0.64
1:G:333:VAL:HG21	1:G:338:ILE:HD11	1.80	0.64
1:A:469:PRO:O	1:A:470:ASP:HB2	1.98	0.63
1:E:156:ASN:OD1	1:E:158:ASN:HB2	1.98	0.63
1:E:363:HIS:CG	3:E:670:HOH:O	2.50	0.63
1:G:50:TRP:O	1:G:70:ARG:NH2	2.32	0.63
1:C:361:ILE:HG23	1:C:371:LEU:HD13	1.81	0.63
1:J:97:PRO:O	1:J:110:ASP:N	2.32	0.63
1:B:29:ALA:HB2	1:B:37:VAL:HG21	1.82	0.62
1:L:96:THR:O	1:L:286:LYS:NZ	2.32	0.62
1:J:150:ARG:NH2	3:J:601:HOH:O	2.31	0.62
1:J:95:ASN:OD1	1:J:95:ASN:N	2.33	0.61
1:I:326:ILE:HG12	1:I:333:VAL:HG21	1.81	0.61
1:G:146:GLY:O	1:G:150:ARG:HG3	2.00	0.61
1:A:169:PHE:CE1	1:A:184:ARG:NH2	2.64	0.60
1:H:139:VAL:O	1:H:140:LYS:HB2	2.00	0.60
1:J:158:ASN:O	1:J:159:LEU:HD22	2.01	0.60
1:A:30:HIS:CE1	1:K:64:GLU:OE2	2.54	0.60
1:E:361:ILE:HG23	1:E:371:LEU:HD13	1.84	0.60
1:D:361:ILE:HG23	1:D:371:LEU:HD13	1.84	0.60
1:J:394:GLN:NE2	1:J:398:ARG:NH2	2.50	0.60
1:F:334:THR:O	1:F:335:ASP:HB2	2.01	0.60
1:A:361:ILE:HG23	1:A:371:LEU:HD13	1.84	0.59
1:B:40:VAL:HG12	1:B:41:ASP:N	2.17	0.59
1:E:339:ALA:HB3	1:E:416:ILE:HD13	1.84	0.59
1:C:25:CYS:HB3	1:C:37:VAL:HG11	1.84	0.59
1:B:66:VAL:O	1:B:70:ARG:N	2.30	0.59
1:H:134:LYS:HE3	1:H:168:GLU:OE1	2.02	0.59
1:I:361:ILE:HG23	1:I:371:LEU:HD13	1.84	0.59
1:D:139:VAL:HG23	1:D:139:VAL:O	2.03	0.59
1:G:59:GLU:OE2	1:G:173:GLY:N	2.36	0.59
1:L:184:ARG:NH1	3:L:601:HOH:O	2.35	0.59
1:J:8:LYS:HE3	1:J:204:ARG:CZ	2.33	0.59
1:J:159:LEU:HD22	1:J:159:LEU:N	2.14	0.59
1:B:363:HIS:CD2	3:B:611:HOH:O	2.55	0.58
1:B:440:PRO:CB	1:F:151:GLU:HG3	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LYS:NZ	3:B:604:HOH:O	2.36	0.58
1:D:132:VAL:HG22	1:D:164:LEU:HB2	1.85	0.58
1:J:87:ALA:O	1:J:129:LYS:NZ	2.27	0.58
1:G:207:GLU:OE2	1:G:212:ARG:HG2	2.04	0.58
1:H:25:CYS:HB3	1:H:37:VAL:HG11	1.85	0.57
1:J:123:GLN:HG2	1:J:124:TYR:CD2	2.38	0.57
1:B:52:SER:N	1:B:70:ARG:NH2	2.53	0.57
1:E:363:HIS:CD2	3:E:670:HOH:O	2.57	0.57
1:L:132:VAL:HG13	1:L:164:LEU:HB2	1.87	0.57
1:F:470:ASP:OD1	1:F:471:GLN:N	2.38	0.57
1:K:156:ASN:OD1	1:K:158:ASN:HB2	2.03	0.57
1:L:50:TRP:O	1:L:70:ARG:NH1	2.38	0.57
1:B:50:TRP:HB3	1:B:76:PHE:CD2	2.40	0.56
1:H:101:TYR:N	1:H:105:LYS:HG3	2.20	0.56
1:G:398:ARG:HG3	1:G:399:LEU:HG	1.88	0.56
1:I:339:ALA:HB3	1:I:416:ILE:HD13	1.87	0.56
1:I:227:LYS:HE3	1:I:231:ASN:HD21	1.71	0.56
1:F:46:LYS:NZ	3:F:606:HOH:O	2.38	0.56
1:B:76:PHE:CD1	1:B:76:PHE:N	2.73	0.56
1:C:414:HIS:NE2	1:C:438:GLN:OE1	2.39	0.56
1:I:46:LYS:NZ	3:I:601:HOH:O	2.33	0.56
1:A:139:VAL:CG2	1:A:228:LEU:HD13	2.36	0.55
1:J:169:PHE:CD2	1:J:184:ARG:HG3	2.39	0.55
1:J:169:PHE:CD2	1:J:184:ARG:CG	2.89	0.55
1:I:156:ASN:OD1	1:I:158:ASN:HB2	2.07	0.55
1:A:169:PHE:HE1	1:A:184:ARG:HH21	1.47	0.55
1:E:193:PRO:O	1:E:197:GLN:HG3	2.06	0.55
1:B:75:PHE:CD1	1:B:75:PHE:N	2.73	0.55
1:B:113:TYR:O	1:B:117:VAL:HG23	2.06	0.55
1:L:357:ALA:HA	1:L:419:LEU:HD13	1.88	0.55
1:B:74:LEU:C	1:B:75:PHE:CD1	2.85	0.54
1:L:100:MET:C	1:L:101:TYR:CD1	2.85	0.54
1:A:339:ALA:HB3	1:A:416:ILE:HD13	1.88	0.54
1:G:184:ARG:HD3	1:H:264:TYR:HB2	1.89	0.54
1:H:146:GLY:O	1:H:150:ARG:HB2	2.07	0.54
1:H:333:VAL:HA	1:H:336:LYS:HD2	1.90	0.54
1:I:8:LYS:CE	1:I:204:ARG:HE	2.21	0.54
1:D:103:ARG:HE	1:D:104:GLY:H	1.56	0.54
1:E:25:CYS:HB3	1:E:37:VAL:CG1	2.36	0.54
1:G:184:ARG:HD3	1:H:264:TYR:CB	2.37	0.54
1:I:8:LYS:HE2	1:I:204:ARG:HE	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:339:ALA:HB3	1:J:416:ILE:HD13	1.89	0.54
1:K:25:CYS:HB3	1:K:37:VAL:HG11	1.88	0.54
1:A:357:ALA:HA	1:A:419:LEU:HD13	1.90	0.54
1:B:361:ILE:HG23	1:B:371:LEU:HD13	1.88	0.54
1:F:101:TYR:CD1	1:F:101:TYR:C	2.85	0.54
1:J:138:PRO:O	1:J:138:PRO:HG2	2.08	0.54
1:J:361:ILE:HG23	1:J:371:LEU:HD13	1.89	0.54
1:I:10:SER:HA	1:I:35:ILE:HD13	1.90	0.54
1:H:159:LEU:HD13	1:H:161:PHE:HE2	1.73	0.54
1:B:137:VAL:HG12	1:B:137:VAL:O	2.08	0.54
1:G:136:THR:OG1	2:G:500:UDX:H2'1	2.08	0.54
1:I:324:LYS:HE3	1:I:328:GLU:HG2	1.89	0.54
1:J:152:ALA:C	1:J:154:LYS:N	2.65	0.54
1:C:132:VAL:HG22	1:C:164:LEU:HB2	1.88	0.53
1:K:68:ALA:O	1:K:72:ARG:NH2	2.41	0.53
1:B:339:ALA:HB3	1:B:416:ILE:HD13	1.89	0.53
1:E:99:LYS:O	1:E:100:MET:HG3	2.07	0.53
1:H:334:THR:O	1:H:335:ASP:HB2	2.08	0.53
1:I:357:ALA:HA	1:I:419:LEU:HD13	1.89	0.53
1:K:361:ILE:HG23	1:K:371:LEU:HD13	1.90	0.53
1:L:86:GLU:HB2	3:L:615:HOH:O	2.09	0.53
1:I:434:HIS:HB2	1:I:460:PHE:CE1	2.44	0.53
1:G:337:LYS:NZ	3:G:605:HOH:O	2.41	0.53
1:F:23:PRO:HB3	1:F:176:MET:CE	2.38	0.53
1:F:414:HIS:NE2	1:F:438:GLN:OE1	2.42	0.53
1:K:137:VAL:HG12	1:K:137:VAL:O	2.09	0.53
1:E:134:LYS:HE3	1:E:168:GLU:OE1	2.09	0.52
1:H:46:LYS:NZ	3:H:607:HOH:O	2.42	0.52
1:A:264:TYR:HB2	1:B:184:ARG:HD3	1.92	0.52
1:L:439:HIS:HA	1:L:440:PRO:C	2.34	0.52
1:A:166:ASN:ND2	1:A:186:LEU:O	2.41	0.52
1:E:401:THR:HG23	3:E:668:HOH:O	2.10	0.52
1:I:324:LYS:HE3	1:I:328:GLU:CG	2.40	0.52
1:B:132:VAL:HG22	1:B:164:LEU:HB2	1.92	0.51
1:B:373:VAL:HB	1:B:383:MET:HE1	1.92	0.51
1:A:191:SER:HB3	3:A:679:HOH:O	2.11	0.51
1:I:137:VAL:HG12	1:I:137:VAL:O	2.10	0.51
1:D:107:MET:HE3	1:D:293:TYR:HB2	1.92	0.51
1:E:357:ALA:HA	1:E:419:LEU:HD13	1.93	0.51
1:K:334:THR:O	1:K:335:ASP:CB	2.59	0.51
1:I:139:VAL:O	1:I:140:LYS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:327:ALA:O	1:J:2:THR:HG22	2.11	0.51
1:K:471:GLN:O	1:K:471:GLN:HG2	2.11	0.51
1:J:159:LEU:N	1:J:159:LEU:CD2	2.74	0.51
1:J:333:VAL:HG23	1:J:369:ALA:HB2	1.93	0.51
1:A:25:CYS:HB3	1:A:37:VAL:CG1	2.41	0.51
1:B:29:ALA:HB2	1:B:37:VAL:CG2	2.41	0.51
1:B:100:MET:C	1:B:105:LYS:HG3	2.35	0.51
1:D:8:LYS:HD2	1:D:204:ARG:CZ	2.41	0.51
1:F:361:ILE:HG23	1:F:371:LEU:HD13	1.93	0.51
1:L:373:VAL:HB	1:L:383:MET:HE1	1.93	0.51
1:F:339:ALA:HB3	1:F:416:ILE:HD13	1.91	0.50
1:H:134:LYS:NZ	1:H:166:ASN:O	2.44	0.50
1:I:326:ILE:HG23	1:I:333:VAL:HG23	1.93	0.50
1:G:132:VAL:HG22	1:G:164:LEU:HB2	1.94	0.50
1:G:361:ILE:HG23	1:G:371:LEU:HD13	1.92	0.50
1:G:326:ILE:HD13	1:G:367:GLU:OE2	2.11	0.50
1:G:373:VAL:HB	1:G:383:MET:HE1	1.92	0.50
1:L:207:GLU:OE2	1:L:212:ARG:HD3	2.11	0.50
1:K:169:PHE:CE1	1:K:184:ARG:NH1	2.80	0.50
1:F:398:ARG:HG3	1:F:399:LEU:HG	1.92	0.50
1:E:184:ARG:HB3	1:F:264:TYR:HB3	1.94	0.50
1:L:100:MET:C	1:L:105:LYS:HG3	2.37	0.49
1:A:134:LYS:HE3	1:A:168:GLU:OE1	2.12	0.49
1:A:395:ASP:OD1	1:A:398:ARG:NH2	2.43	0.49
1:F:25:CYS:HB3	1:F:37:VAL:CG1	2.43	0.49
1:B:99:LYS:O	1:B:106:GLY:N	2.44	0.49
1:C:414:HIS:CE1	1:C:438:GLN:OE1	2.65	0.49
1:F:357:ALA:HA	1:F:419:LEU:HD13	1.94	0.49
1:K:150:ARG:O	1:K:154:LYS:HG3	2.12	0.49
1:I:207:GLU:OE2	1:I:212:ARG:HD3	2.12	0.49
1:G:374:TYR:CE2	1:G:406:PRO:HG3	2.48	0.49
1:J:50:TRP:O	1:J:70:ARG:NH1	2.44	0.49
1:C:95:ASN:OD1	2:C:500:UDX:H61	2.13	0.49
1:G:68:ALA:O	1:G:72:ARG:NH1	2.46	0.49
1:L:333:VAL:HA	1:L:336:LYS:HD2	1.93	0.49
1:C:139:VAL:HG13	1:C:139:VAL:O	2.13	0.49
1:C:129:LYS:HE2	3:C:614:HOH:O	2.12	0.49
1:D:9:VAL:HG13	1:D:88:ASP:HB2	1.94	0.49
1:F:227:LYS:HE3	1:F:231:ASN:HD21	1.77	0.49
1:B:40:VAL:CG1	1:B:41:ASP:N	2.75	0.49
1:I:25:CYS:HB3	1:I:37:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:GLN:HG3	1:E:311:ILE:HD12	1.95	0.48
1:L:23:PRO:HB3	1:L:176:MET:CE	2.41	0.48
1:L:100:MET:HB2	1:L:101:TYR:CE1	2.48	0.48
1:B:69:ALA:HB2	3:B:682:HOH:O	2.12	0.48
1:D:285:GLN:HG3	1:D:311:ILE:HD12	1.95	0.48
1:J:152:ALA:C	1:J:154:LYS:H	2.21	0.48
1:B:102:GLY:HA3	1:D:367:GLU:OE1	2.14	0.48
1:I:23:PRO:HB3	1:I:176:MET:CE	2.39	0.48
1:I:197:GLN:O	1:I:201:GLU:HG2	2.14	0.48
1:J:25:CYS:HB3	1:J:37:VAL:CG1	2.39	0.48
1:C:395:ASP:OD1	1:C:398:ARG:NH1	2.46	0.48
1:C:212:ARG:NH2	1:C:215:ILE:O	2.46	0.48
1:H:326:ILE:HD13	1:H:367:GLU:OE2	2.14	0.48
1:I:134:LYS:HE3	1:I:168:GLU:OE2	2.14	0.48
1:B:75:PHE:C	1:B:76:PHE:CD1	2.93	0.47
1:F:238[B]:ILE:HD11	1:F:272:PHE:CD2	2.49	0.47
1:J:137:VAL:O	1:J:137:VAL:HG12	2.13	0.47
1:D:134:LYS:HE3	1:D:168:GLU:OE1	2.14	0.47
1:H:357:ALA:HA	1:H:419:LEU:HD13	1.95	0.47
1:I:264:TYR:HB3	1:J:184:ARG:HB3	1.96	0.47
1:J:340:ILE:HD13	1:J:417:VAL:CG1	2.44	0.47
1:C:357:ALA:HA	1:C:419:LEU:HD13	1.96	0.47
1:K:357:ALA:HA	1:K:419:LEU:HD13	1.96	0.47
1:L:99:LYS:HD3	1:L:108:ALA:HB3	1.96	0.47
1:B:101:TYR:N	1:B:105:LYS:HG3	2.30	0.47
1:J:15:VAL:HA	1:J:40:VAL:HG23	1.97	0.47
1:C:373:VAL:HB	1:C:383:MET:HE1	1.96	0.47
1:D:334:THR:HG22	1:D:335:ASP:OD1	2.14	0.47
1:G:52:SER:O	1:G:70:ARG:NH1	2.39	0.47
1:A:373:VAL:HB	1:A:383:MET:HE1	1.97	0.47
1:K:302:GLN:H	1:K:302:GLN:CD	2.23	0.47
1:J:110:ASP:OD2	1:J:112:LYS:CB	2.63	0.47
1:C:412:GLY:O	1:C:438:GLN:NE2	2.48	0.46
1:H:25:CYS:HB3	1:H:37:VAL:CG1	2.45	0.46
1:F:132:VAL:HG22	1:F:164:LEU:HB2	1.97	0.46
1:L:184:ARG:HH12	1:L:230:ALA:HB1	1.81	0.46
1:G:303:VAL:HG13	1:H:243:SER:HB2	1.97	0.46
1:G:357:ALA:HA	1:G:419:LEU:HD13	1.97	0.46
1:C:274:GLN:HG2	3:C:713:HOH:O	2.16	0.46
1:I:27:MET:HG2	1:I:179:LEU:HB3	1.98	0.46
1:I:184:ARG:NH1	1:J:261:ALA:O	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:347:LYS:HE2	3:K:668:HOH:O	2.15	0.46
1:C:207:GLU:OE2	1:C:212:ARG:HD3	2.16	0.46
1:D:109:PRO:CG	1:D:139:VAL:HG21	2.27	0.46
1:H:92:ILE:HD12	1:H:145:ILE:HD13	1.98	0.46
1:J:158:ASN:N	1:J:158:ASN:OD1	2.49	0.46
1:C:25:CYS:HB3	1:C:37:VAL:CG1	2.45	0.46
1:J:9:VAL:HG11	1:J:205:ILE:HD11	1.98	0.46
1:L:285:GLN:HG3	1:L:311:ILE:HD12	1.97	0.46
1:B:184:ARG:NH1	3:B:607:HOH:O	2.48	0.45
1:G:32:CYS:C	3:G:620:HOH:O	2.58	0.45
1:A:207:GLU:OE2	1:A:212:ARG:HD3	2.16	0.45
1:K:127:GLY:N	1:K:159:LEU:HD22	2.31	0.45
1:A:30:HIS:NE2	1:K:64:GLU:OE2	2.50	0.45
1:D:340:ILE:HG21	1:D:361:ILE:HD11	1.97	0.45
1:E:64:GLU:OE2	1:H:427:GLU:HB2	2.17	0.45
1:K:373:VAL:HB	1:K:383:MET:HE1	1.98	0.45
1:L:99:LYS:CG	1:L:108:ALA:O	2.64	0.45
1:F:461:ARG:NH1	3:F:612:HOH:O	2.48	0.45
1:G:436:ASP:HB2	3:G:616:HOH:O	2.17	0.45
1:K:262:VAL:HA	1:L:184:ARG:HH22	1.82	0.45
1:A:188:GLY:HA2	1:A:218:THR:O	2.17	0.45
1:C:129:LYS:NZ	3:C:614:HOH:O	2.49	0.45
1:C:140:LYS:HA	1:C:143:GLU:OE2	2.16	0.45
1:B:453:LYS:O	1:B:457:GLU:HG3	2.16	0.45
1:E:86:GLU:HB3	3:E:632:HOH:O	2.15	0.45
1:E:261:ALA:O	1:F:184:ARG:NH1	2.46	0.45
1:J:207:GLU:OE2	1:J:212:ARG:HD3	2.17	0.45
1:K:333:VAL:CG2	1:K:338:ILE:HD11	2.45	0.45
1:E:98:THR:HG21	1:E:106:GLY:C	2.42	0.45
1:G:32:CYS:CA	3:G:620:HOH:O	2.64	0.45
1:B:470:ASP:OD1	1:B:470:ASP:N	2.50	0.44
1:D:299:ASN:O	1:D:301:PRO:HD3	2.17	0.44
1:G:139:VAL:HG21	1:G:290:SER:OG	2.16	0.44
1:G:333:VAL:CG2	1:G:338:ILE:HD11	2.45	0.44
1:B:69:ALA:HA	1:B:72:ARG:HD3	1.98	0.44
1:L:340:ILE:HG21	1:L:361:ILE:HD11	1.98	0.44
1:C:146:GLY:O	1:C:150:ARG:HG3	2.17	0.44
1:I:157:GLU:O	1:I:160:LYS:NZ	2.47	0.44
1:B:117:VAL:O	1:B:121:ILE:HG13	2.18	0.44
1:D:212:ARG:NH1	1:D:215:ILE:O	2.51	0.44
1:L:201:GLU:OE1	1:L:201:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:MET:HG2	2:F:500:UDX:C2	2.48	0.44
1:E:272:PHE:CE1	1:F:267:ARG:HD2	2.52	0.44
1:I:303:VAL:HG13	1:J:243:SER:HB2	2.00	0.44
1:I:376:PRO:O	1:I:377:LYS:HD2	2.18	0.44
1:J:132:VAL:HG22	1:J:164:LEU:HB2	1.99	0.44
1:L:20:VAL:O	1:L:24:THR:OG1	2.31	0.44
1:A:394:GLN:O	1:A:398:ARG:HG3	2.17	0.44
1:B:52:SER:N	1:B:70:ARG:HH22	2.16	0.44
1:A:337:LYS:HE2	1:A:409:ALA:O	2.18	0.44
1:E:326:ILE:HD13	1:E:367:GLU:OE2	2.18	0.44
1:K:139:VAL:CG2	1:K:228:LEU:HD13	2.48	0.44
1:L:176:MET:HE2	1:L:176:MET:HA	2.00	0.44
1:C:129:LYS:CE	3:C:614:HOH:O	2.64	0.43
1:B:101:TYR:CE2	1:D:368:HIS:CE1	3.06	0.43
1:D:128:PRO:HA	1:D:160:LYS:O	2.18	0.43
1:E:149:LEU:HD13	1:E:161:PHE:CG	2.54	0.43
1:L:302:GLN:CD	1:L:302:GLN:H	2.26	0.43
1:G:261:ALA:O	1:H:184:ARG:NH1	2.44	0.43
1:L:434:HIS:HB2	1:L:460:PHE:CE2	2.53	0.43
1:C:23:PRO:HB3	1:C:176:MET:CE	2.41	0.43
1:H:99:LYS:HB3	1:H:99:LYS:HE2	1.79	0.43
1:K:439:HIS:HA	1:K:440:PRO:C	2.43	0.43
1:F:415:ALA:HA	1:F:442:ALA:O	2.18	0.43
1:G:134:LYS:HE3	1:G:168:GLU:OE1	2.18	0.43
1:I:49:GLU:OE1	1:I:56:PRO:HB3	2.19	0.43
1:B:74:LEU:HG	1:B:76:PHE:HE1	1.84	0.43
1:G:23:PRO:HB3	1:G:176:MET:CE	2.48	0.43
1:H:392:SER:OG	1:H:395:ASP:OD2	2.35	0.43
1:J:110:ASP:OD2	1:J:112:LYS:HB3	2.19	0.43
1:L:170:LEU:C	1:L:170:LEU:CD1	2.85	0.43
1:B:299:ASN:C	1:B:301:PRO:HD3	2.44	0.43
1:D:357:ALA:HA	1:D:419:LEU:HD13	2.00	0.43
1:B:357:ALA:HA	1:B:419:LEU:HD13	2.01	0.43
1:C:334:THR:HG22	1:C:368:HIS:HB2	1.99	0.43
1:G:333:VAL:O	1:G:333:VAL:HG22	2.19	0.43
1:K:404:SER:HA	3:K:695:HOH:O	2.18	0.43
1:G:139:VAL:O	1:G:140:LYS:HB2	2.18	0.43
1:J:49:GLU:OE1	1:J:56:PRO:HB3	2.19	0.43
1:H:139:VAL:HG21	1:H:290:SER:OG	2.19	0.43
1:H:207:GLU:OE2	1:H:212:ARG:HD3	2.19	0.42
1:D:468:SER:HA	1:D:469:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:352:THR:OG1	1:H:386:ASP:OD2	2.32	0.42
1:J:150:ARG:O	1:J:154:LYS:HB2	2.19	0.42
1:B:326:ILE:HD13	1:B:367:GLU:OE2	2.19	0.42
1:C:53:ASP:OD1	1:C:53:ASP:N	2.51	0.42
1:D:333:VAL:HA	1:D:336:LYS:HD2	2.01	0.42
1:K:46:LYS:NZ	3:K:610:HOH:O	2.48	0.42
1:A:119:ARG:NE	3:A:606:HOH:O	2.48	0.42
1:A:326:ILE:HD13	1:A:367:GLU:OE1	2.19	0.42
1:D:359:HIS:HB3	3:D:725:HOH:O	2.19	0.42
1:C:439:HIS:HA	1:C:440:PRO:C	2.44	0.42
1:J:285:GLN:HG3	1:J:311:ILE:HD12	2.02	0.42
1:D:207:GLU:OE2	1:D:212:ARG:HD3	2.20	0.42
1:G:16:GLY:O	1:G:21:GLY:HA3	2.20	0.42
1:K:415:ALA:HA	1:K:442:ALA:O	2.20	0.42
1:L:25:CYS:HB3	1:L:37:VAL:HG11	2.02	0.42
1:B:101:TYR:CD1	1:B:101:TYR:C	2.97	0.42
1:D:284:PHE:CE2	2:D:501:UDX:H5A1	2.55	0.42
1:D:319:ARG:HD3	3:D:716:HOH:O	2.20	0.42
1:G:227:LYS:HE3	1:G:231:ASN:HD21	1.85	0.42
1:G:338:ILE:HB	1:G:371:LEU:HD23	2.02	0.42
1:I:267:ARG:HD2	1:J:272:PHE:CE1	2.54	0.42
1:I:394:GLN:HG2	1:I:398:ARG:NH1	2.34	0.42
1:K:27:MET:HE2	1:K:176:MET:HE3	2.02	0.42
1:B:207:GLU:OE2	1:B:212:ARG:HG2	2.20	0.42
1:C:137:VAL:HG21	1:C:286:LYS:HD3	2.01	0.42
1:F:100:MET:HE2	1:F:100:MET:HB3	1.86	0.42
1:F:218:THR:OG1	1:F:219:ASN:N	2.52	0.42
1:L:274:GLN:HG2	3:L:668:HOH:O	2.20	0.42
1:D:376:PRO:O	1:D:377:LYS:HD2	2.19	0.42
1:J:175:ALA:HB3	1:J:176:MET:HE2	2.02	0.42
1:D:99:LYS:HG3	1:D:108:ALA:O	2.20	0.42
1:E:398:ARG:HG3	1:E:399:LEU:HG	2.01	0.42
1:G:32:CYS:HA	3:G:620:HOH:O	2.19	0.42
1:H:376:PRO:HD2	1:H:422:TRP:CE2	2.55	0.42
1:K:101:TYR:CD1	1:K:101:TYR:C	2.97	0.42
1:E:107:MET:HE3	1:E:293:TYR:HB2	2.01	0.41
1:J:340:ILE:HD11	1:J:371:LEU:HD22	2.02	0.41
1:D:3:ASP:HA	1:D:197:GLN:HE22	1.84	0.41
1:D:299:ASN:O	1:D:301:PRO:CD	2.69	0.41
1:E:113:TYR:HB3	2:E:500:UDX:H51	2.03	0.41
1:I:42:MET:HG2	2:I:500:UDX:C2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:8:LYS:HG3	1:J:204:ARG:NH1	2.36	0.41
1:A:415:ALA:HA	1:A:442:ALA:O	2.20	0.41
1:B:134:LYS:HE3	1:B:168:GLU:OE1	2.19	0.41
1:E:155:ASN:HB2	3:E:660:HOH:O	2.19	0.41
1:F:373:VAL:HB	1:F:383:MET:HE1	2.02	0.41
1:G:25:CYS:HB3	1:G:37:VAL:CG1	2.47	0.41
1:A:438:GLN:HE21	1:A:438:GLN:HA	1.84	0.41
1:A:468:SER:HA	1:A:469:PRO:HD3	1.85	0.41
1:D:107:MET:HB3	1:D:293:TYR:HB2	2.03	0.41
1:I:302:GLN:OE1	1:J:316:TRP:CD1	2.74	0.41
1:I:378:VAL:HA	3:I:606:HOH:O	2.20	0.41
1:J:140:LYS:HA	1:J:143:GLU:OE1	2.19	0.41
1:H:227:LYS:HE3	1:H:231:ASN:HD21	1.84	0.41
1:F:434:HIS:HB2	1:F:460:PHE:CE2	2.56	0.41
1:G:59:GLU:HG2	1:G:175:ALA:HB3	2.02	0.41
1:A:333:VAL:HA	1:A:336:LYS:HD2	2.03	0.41
1:A:352:THR:OG1	1:A:386:ASP:OD2	2.36	0.41
1:C:13:VAL:HG22	1:C:38:THR:HB	2.02	0.41
1:C:264:TYR:HB3	1:D:184:ARG:HB3	2.03	0.41
1:F:176:MET:HA	1:F:176:MET:HE2	2.02	0.41
1:G:70:ARG:HA	1:G:74:LEU:O	2.20	0.41
1:L:212:ARG:NH1	1:L:215:ILE:O	2.51	0.41
1:D:113:TYR:CG	2:D:500:UDX:H51	2.56	0.41
1:A:138:PRO:HG3	1:A:167:PRO:HB3	2.02	0.41
1:C:77:SER:OG	1:C:78:SER:N	2.54	0.41
1:D:175:ALA:HB3	1:D:176:MET:HE2	2.01	0.41
1:D:241:ILE:HD12	1:D:241:ILE:HA	1.96	0.41
1:J:151:GLU:O	1:J:154:LYS:N	2.52	0.41
1:K:8:LYS:HG3	1:K:204:ARG:HE	1.86	0.41
1:K:188:GLY:HA2	1:K:218:THR:O	2.21	0.41
1:K:383:MET:HE3	1:K:383:MET:HB3	1.89	0.41
1:F:101:TYR:C	1:F:101:TYR:HD1	2.28	0.41
1:L:155:ASN:HB2	3:L:638:HOH:O	2.20	0.41
1:L:227:LYS:HE3	1:L:231:ASN:HD21	1.86	0.41
1:A:468:SER:C	1:A:470:ASP:H	2.29	0.40
1:C:184:ARG:NH1	1:D:261:ALA:O	2.49	0.40
1:H:108:ALA:HA	1:H:109:PRO:HD3	1.93	0.40
1:A:58:TYR:CE1	1:A:377:LYS:HE3	2.56	0.40
1:G:376:PRO:HD2	1:G:422:TRP:CE2	2.56	0.40
1:J:228:LEU:HD11	1:J:291:LEU:HB2	2.04	0.40
1:D:394:GLN:O	1:D:398:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:ALA:HA	1:D:442:ALA:O	2.22	0.40
1:E:227:LYS:HE3	1:E:231:ASN:HD21	1.85	0.40
1:F:40:VAL:HA	1:F:77:SER:O	2.21	0.40
1:H:338:ILE:HB	1:H:371:LEU:HD23	2.04	0.40
1:H:392:SER:HG	1:H:395:ASP:CG	2.27	0.40
1:J:417:VAL:O	1:J:417:VAL:HG13	2.22	0.40
1:K:107:MET:HE3	1:K:293:TYR:HD1	1.87	0.40
1:L:212:ARG:NH1	1:L:215:ILE:HB	2.36	0.40
1:B:64:GLU:HG2	1:L:427:GLU:OE1	2.21	0.40
1:B:383:MET:HE3	1:B:383:MET:HB3	1.88	0.40
1:C:285:GLN:HG3	1:C:311:ILE:HD12	2.03	0.40
1:D:84:ILE:O	1:D:129:LYS:HE3	2.21	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	461/481 (96%)	444 (96%)	17 (4%)	0	100	100
1	B	462/481 (96%)	444 (96%)	18 (4%)	0	100	100
1	C	462/481 (96%)	446 (96%)	16 (4%)	0	100	100
1	D	467/481 (97%)	448 (96%)	19 (4%)	0	100	100
1	E	459/481 (95%)	444 (97%)	15 (3%)	0	100	100
1	F	466/481 (97%)	448 (96%)	18 (4%)	0	100	100
1	G	462/481 (96%)	448 (97%)	14 (3%)	0	100	100
1	H	463/481 (96%)	446 (96%)	17 (4%)	0	100	100
1	I	462/481 (96%)	449 (97%)	13 (3%)	0	100	100
1	J	451/481 (94%)	437 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	464/481 (96%)	451 (97%)	13 (3%)	0	100	100
1	L	463/481 (96%)	449 (97%)	14 (3%)	0	100	100
All	All	5542/5772 (96%)	5354 (97%)	188 (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	386/399 (97%)	383 (99%)	3 (1%)	73	81
1	B	387/399 (97%)	385 (100%)	2 (0%)	81	87
1	C	387/399 (97%)	384 (99%)	3 (1%)	73	81
1	D	391/399 (98%)	391 (100%)	0	100	100
1	E	387/399 (97%)	387 (100%)	0	100	100
1	F	390/399 (98%)	388 (100%)	2 (0%)	81	87
1	G	387/399 (97%)	385 (100%)	2 (0%)	81	87
1	H	388/399 (97%)	387 (100%)	1 (0%)	86	91
1	I	387/399 (97%)	387 (100%)	0	100	100
1	J	383/399 (96%)	377 (98%)	6 (2%)	55	68
1	K	389/399 (98%)	387 (100%)	2 (0%)	81	87
1	L	387/399 (97%)	378 (98%)	9 (2%)	44	57
All	All	4649/4788 (97%)	4619 (99%)	30 (1%)	78	85

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	LYS
1	A	184	ARG
1	A	438	GLN
1	B	103	ARG

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Mol	Chain	Res	Type
1	B	319	ARG
1	C	78	SER
1	C	100	MET
1	C	184	ARG
1	F	120	THR
1	F	159	LEU
1	G	153	GLN
1	G	159	LEU
1	H	435	ASN
1	J	95	ASN
1	J	154	LYS
1	J	155	ASN
1	J	158	ASN
1	J	333	VAL
1	J	431	SER
1	K	151	GLU
1	K	470	ASP
1	L	24	THR
1	L	103	ARG
1	L	114	VAL
1	L	132	VAL
1	L	137	VAL
1	L	139	VAL
1	L	162	GLN
1	L	170	LEU
1	L	418	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	GLN
1	A	359	HIS
1	A	368	HIS
1	A	394	GLN
1	A	438	GLN
1	B	30	HIS
1	B	236	GLN
1	B	299	ASN
1	B	308	GLN
1	B	368	HIS
1	B	434	HIS
1	C	166	ASN

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Mol	Chain	Res	Type
1	C	208	ASN
1	C	231	ASN
1	C	236	GLN
1	C	299	ASN
1	C	302	GLN
1	C	382	GLN
1	C	434	HIS
1	D	162	GLN
1	D	166	ASN
1	D	197	GLN
1	D	285	GLN
1	D	308	GLN
1	E	181	ASN
1	E	213	ASN
1	E	231	ASN
1	E	274	GLN
1	E	302	GLN
1	E	368	HIS
1	F	166	ASN
1	F	208	ASN
1	F	452	GLN
1	G	231	ASN
1	G	299	ASN
1	G	414	HIS
1	H	30	HIS
1	H	231	ASN
1	H	236	GLN
1	H	308	GLN
1	I	30	HIS
1	I	162	GLN
1	I	231	ASN
1	I	274	GLN
1	I	308	GLN
1	J	158	ASN
1	J	162	GLN
1	J	274	GLN
1	J	394	GLN
1	J	414	HIS
1	K	158	ASN
1	K	231	ASN
1	L	166	ASN
1	L	208	ASN

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Mol	Chain	Res	Type
1	L	231	ASN
1	L	382	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](#)

24 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	E	500	-	35,36,36	1.05	2 (5%)	52,55,55	1.43	6 (11%)
2	UDX	K	501	-	35,36,36	1.07	3 (8%)	52,55,55	1.38	7 (13%)
2	UDX	G	500	-	35,36,36	1.13	4 (11%)	52,55,55	1.35	5 (9%)
2	UDX	D	500	-	35,36,36	1.05	4 (11%)	52,55,55	1.39	6 (11%)
2	UDX	I	500	-	35,36,36	1.16	4 (11%)	52,55,55	1.40	5 (9%)
2	UDX	K	500	-	35,36,36	1.09	4 (11%)	52,55,55	1.41	5 (9%)
2	UDX	C	500	-	35,36,36	1.05	2 (5%)	52,55,55	1.39	4 (7%)
2	UDX	A	501	-	35,36,36	1.09	3 (8%)	52,55,55	1.44	6 (11%)
2	UDX	A	500	-	35,36,36	1.03	3 (8%)	52,55,55	1.40	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UDX	L	501	-	35,36,36	1.12	5 (14%)	52,55,55	1.39	6 (11%)
2	UDX	L	500	-	35,36,36	1.12	4 (11%)	52,55,55	1.47	5 (9%)
2	UDX	F	500	-	35,36,36	1.14	6 (17%)	52,55,55	1.40	4 (7%)
2	UDX	I	501	-	35,36,36	1.10	5 (14%)	52,55,55	1.47	6 (11%)
2	UDX	D	501	-	35,36,36	1.17	5 (14%)	52,55,55	1.46	5 (9%)
2	UDX	E	501	-	35,36,36	1.12	4 (11%)	52,55,55	1.44	5 (9%)
2	UDX	H	501	-	35,36,36	1.13	4 (11%)	52,55,55	1.38	6 (11%)
2	UDX	C	501	-	35,36,36	1.19	4 (11%)	52,55,55	1.39	6 (11%)
2	UDX	H	500	-	35,36,36	1.06	2 (5%)	52,55,55	1.35	5 (9%)
2	UDX	G	501	-	35,36,36	1.13	4 (11%)	52,55,55	1.44	6 (11%)
2	UDX	F	501	-	35,36,36	1.14	4 (11%)	52,55,55	1.54	7 (13%)
2	UDX	B	501	-	35,36,36	1.24	4 (11%)	52,55,55	1.42	6 (11%)
2	UDX	B	500	-	35,36,36	1.11	4 (11%)	52,55,55	1.45	6 (11%)
2	UDX	J	501	-	35,36,36	1.14	6 (17%)	52,55,55	1.42	5 (9%)
2	UDX	J	500	-	35,36,36	1.13	5 (14%)	52,55,55	1.34	4 (7%)

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	E	500	-	-	5/21/54/54	0/3/3/3
2	UDX	K	501	-	-	5/21/54/54	0/3/3/3
2	UDX	G	500	-	-	4/21/54/54	0/3/3/3
2	UDX	D	500	-	-	4/21/54/54	0/3/3/3
2	UDX	I	500	-	-	4/21/54/54	0/3/3/3
2	UDX	K	500	-	-	5/21/54/54	0/3/3/3
2	UDX	C	500	-	-	4/21/54/54	0/3/3/3
2	UDX	A	501	-	-	5/21/54/54	0/3/3/3
2	UDX	A	500	-	-	5/21/54/54	0/3/3/3
2	UDX	L	501	-	-	5/21/54/54	0/3/3/3
2	UDX	L	500	-	-	3/21/54/54	0/3/3/3
2	UDX	F	500	-	-	4/21/54/54	0/3/3/3
2	UDX	I	501	-	-	3/21/54/54	0/3/3/3
2	UDX	D	501	-	-	5/21/54/54	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDX	E	501	-	-	3/21/54/54	0/3/3/3
2	UDX	H	501	-	-	5/21/54/54	0/3/3/3
2	UDX	C	501	-	-	3/21/54/54	0/3/3/3
2	UDX	H	500	-	-	5/21/54/54	0/3/3/3
2	UDX	G	501	-	-	6/21/54/54	0/3/3/3
2	UDX	F	501	-	-	10/21/54/54	0/3/3/3
2	UDX	B	501	-	-	9/21/54/54	0/3/3/3
2	UDX	B	500	-	-	7/21/54/54	0/3/3/3
2	UDX	J	501	-	-	7/21/54/54	0/3/3/3
2	UDX	J	500	-	-	5/21/54/54	0/3/3/3

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	UDX	PA-O3A	3.24	1.63	1.59
2	C	501	UDX	PB-O3A	3.21	1.63	1.59
2	B	501	UDX	PB-O3A	3.14	1.62	1.59
2	G	501	UDX	PB-O3A	2.95	1.62	1.59
2	F	501	UDX	C4-N3	-2.89	1.33	1.38
2	L	501	UDX	C4-N3	-2.85	1.33	1.38
2	D	501	UDX	C4-N3	-2.80	1.33	1.38
2	C	500	UDX	C4-N3	-2.78	1.33	1.38
2	B	501	UDX	C4-N3	-2.77	1.33	1.38
2	D	501	UDX	PB-O3A	2.76	1.62	1.59
2	K	501	UDX	C4-N3	-2.75	1.33	1.38
2	I	501	UDX	PB-O3A	2.75	1.62	1.59
2	A	501	UDX	PB-O3A	2.75	1.62	1.59
2	H	501	UDX	PB-O3A	2.71	1.62	1.59
2	I	500	UDX	PB-O3A	2.71	1.62	1.59
2	F	500	UDX	C4-N3	-2.69	1.34	1.38
2	I	500	UDX	C4-N3	-2.69	1.34	1.38
2	F	501	UDX	PB-O3A	2.67	1.62	1.59
2	J	501	UDX	PB-O3A	2.65	1.62	1.59
2	H	500	UDX	C4-N3	-2.63	1.34	1.38
2	E	501	UDX	C4-N3	-2.63	1.34	1.38
2	C	501	UDX	C4-N3	-2.62	1.34	1.38
2	J	501	UDX	C4-N3	-2.61	1.34	1.38
2	B	500	UDX	C4-N3	-2.59	1.34	1.38
2	G	500	UDX	C4-N3	-2.55	1.34	1.38
2	J	500	UDX	C4-N3	-2.54	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	UDX	C4-N3	-2.53	1.34	1.38
2	I	501	UDX	C4-N3	-2.53	1.34	1.38
2	F	501	UDX	PA-O3A	2.52	1.62	1.59
2	L	500	UDX	PB-O3A	2.50	1.62	1.59
2	F	500	UDX	PA-O3A	2.46	1.62	1.59
2	A	500	UDX	C4-N3	-2.46	1.34	1.38
2	L	500	UDX	PA-O3A	2.45	1.62	1.59
2	D	501	UDX	C2-N3	-2.45	1.33	1.38
2	K	500	UDX	C4-N3	-2.45	1.34	1.38
2	B	501	UDX	C2-N3	-2.44	1.33	1.38
2	K	501	UDX	C2-N3	-2.42	1.33	1.38
2	J	500	UDX	PA-O3A	2.42	1.62	1.59
2	H	501	UDX	C4-N3	-2.41	1.34	1.38
2	F	501	UDX	C2-N3	-2.41	1.33	1.38
2	B	500	UDX	PA-O3A	2.41	1.62	1.59
2	E	501	UDX	PA-O3A	2.40	1.62	1.59
2	C	501	UDX	PA-O3A	2.39	1.62	1.59
2	G	501	UDX	C4-N3	-2.38	1.34	1.38
2	G	500	UDX	PA-O3A	2.37	1.62	1.59
2	H	501	UDX	PA-O3A	2.35	1.62	1.59
2	A	501	UDX	C2-N3	-2.35	1.33	1.38
2	J	501	UDX	PA-O3A	2.34	1.62	1.59
2	L	501	UDX	PA-O3A	2.33	1.62	1.59
2	J	500	UDX	C2-N1	2.33	1.42	1.38
2	L	500	UDX	C4-N3	-2.33	1.34	1.38
2	F	500	UDX	C2-N3	-2.33	1.33	1.38
2	E	501	UDX	PB-O3A	2.31	1.62	1.59
2	G	501	UDX	PA-O3A	2.31	1.62	1.59
2	D	501	UDX	PA-O3A	2.30	1.62	1.59
2	K	500	UDX	PB-O3A	2.30	1.62	1.59
2	I	500	UDX	C2-N3	-2.30	1.34	1.38
2	G	500	UDX	PB-O3A	2.28	1.62	1.59
2	D	500	UDX	C4-N3	-2.26	1.34	1.38
2	I	501	UDX	PA-O3A	2.26	1.61	1.59
2	C	501	UDX	C2-N3	-2.25	1.34	1.38
2	J	501	UDX	C2-N3	-2.25	1.34	1.38
2	C	500	UDX	C2-N3	-2.25	1.34	1.38
2	F	500	UDX	PB-O3A	2.25	1.61	1.59
2	K	501	UDX	PB-O3A	2.25	1.61	1.59
2	B	500	UDX	PB-O3A	2.24	1.61	1.59
2	F	500	UDX	C2-N1	2.23	1.41	1.38
2	H	500	UDX	C2-N3	-2.22	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	500	UDX	PA-O3A	2.19	1.61	1.59
2	L	501	UDX	C2-N3	-2.19	1.34	1.38
2	L	501	UDX	PB-O3A	2.19	1.61	1.59
2	E	500	UDX	C2-N1	2.18	1.41	1.38
2	H	501	UDX	C5-C4	-2.17	1.39	1.43
2	J	500	UDX	PB-O3A	2.17	1.61	1.59
2	D	501	UDX	C2-N1	2.17	1.41	1.38
2	E	500	UDX	C4-N3	-2.16	1.34	1.38
2	E	501	UDX	C2-N3	-2.15	1.34	1.38
2	B	500	UDX	C2-N3	-2.15	1.34	1.38
2	G	500	UDX	C2-N3	-2.12	1.34	1.38
2	L	500	UDX	C2-N3	-2.12	1.34	1.38
2	K	500	UDX	PA-O3A	2.11	1.61	1.59
2	I	501	UDX	C2-N3	-2.08	1.34	1.38
2	J	500	UDX	C2-N3	-2.06	1.34	1.38
2	I	501	UDX	C6-C5	2.06	1.39	1.35
2	K	500	UDX	C2-N3	-2.05	1.34	1.38
2	D	500	UDX	C6-C5	2.05	1.39	1.35
2	A	500	UDX	C2-N3	-2.05	1.34	1.38
2	D	500	UDX	C2-N3	-2.04	1.34	1.38
2	F	500	UDX	C6-C5	2.03	1.39	1.35
2	L	501	UDX	C6-C5	2.03	1.39	1.35
2	J	501	UDX	C6-C5	2.03	1.39	1.35
2	D	500	UDX	C2-N1	2.02	1.41	1.38
2	A	500	UDX	C2-N1	2.01	1.41	1.38
2	J	501	UDX	C2-N1	2.01	1.41	1.38
2	G	501	UDX	C6-C5	2.01	1.39	1.35

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	501	UDX	C4-N3-C2	-5.68	119.56	126.61
2	D	501	UDX	C4-N3-C2	-5.36	119.95	126.61
2	B	501	UDX	C4-N3-C2	-5.20	120.16	126.61
2	G	501	UDX	C4-N3-C2	-5.16	120.21	126.61
2	J	501	UDX	C4-N3-C2	-5.14	120.23	126.61
2	L	500	UDX	C4-N3-C2	-5.13	120.24	126.61
2	A	501	UDX	C4-N3-C2	-5.10	120.28	126.61
2	A	500	UDX	C4-N3-C2	-5.09	120.29	126.61
2	B	500	UDX	C4-N3-C2	-5.09	120.29	126.61
2	I	500	UDX	C4-N3-C2	-5.04	120.35	126.61
2	K	500	UDX	C4-N3-C2	-5.04	120.36	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	501	UDX	C4-N3-C2	-5.03	120.36	126.61
2	C	501	UDX	C4-N3-C2	-5.03	120.37	126.61
2	F	500	UDX	C4-N3-C2	-5.00	120.41	126.61
2	E	501	UDX	C4-N3-C2	-4.95	120.47	126.61
2	C	500	UDX	C4-N3-C2	-4.91	120.52	126.61
2	D	500	UDX	C4-N3-C2	-4.86	120.58	126.61
2	E	500	UDX	C4-N3-C2	-4.83	120.62	126.61
2	G	500	UDX	C4-N3-C2	-4.75	120.71	126.61
2	L	501	UDX	C4-N3-C2	-4.74	120.73	126.61
2	F	501	UDX	C5-C4-N3	4.73	121.42	114.80
2	D	501	UDX	N3-C2-N1	4.72	121.03	114.89
2	H	500	UDX	C4-N3-C2	-4.70	120.78	126.61
2	H	501	UDX	C4-N3-C2	-4.68	120.80	126.61
2	J	500	UDX	C4-N3-C2	-4.64	120.86	126.61
2	K	501	UDX	C4-N3-C2	-4.61	120.89	126.61
2	I	501	UDX	N3-C2-N1	4.56	120.83	114.89
2	A	500	UDX	N3-C2-N1	4.53	120.79	114.89
2	B	501	UDX	N3-C2-N1	4.52	120.78	114.89
2	J	501	UDX	N3-C2-N1	4.49	120.74	114.89
2	B	500	UDX	N3-C2-N1	4.48	120.72	114.89
2	C	500	UDX	N3-C2-N1	4.42	120.65	114.89
2	L	500	UDX	N3-C2-N1	4.41	120.64	114.89
2	L	501	UDX	N3-C2-N1	4.38	120.59	114.89
2	C	501	UDX	N3-C2-N1	4.35	120.56	114.89
2	A	501	UDX	N3-C2-N1	4.34	120.54	114.89
2	E	501	UDX	N3-C2-N1	4.33	120.52	114.89
2	F	500	UDX	N3-C2-N1	4.28	120.46	114.89
2	I	500	UDX	N3-C2-N1	4.27	120.44	114.89
2	D	500	UDX	N3-C2-N1	4.27	120.44	114.89
2	F	501	UDX	N3-C2-N1	4.25	120.42	114.89
2	E	500	UDX	N3-C2-N1	4.23	120.39	114.89
2	G	501	UDX	N3-C2-N1	4.19	120.34	114.89
2	D	501	UDX	C5-C4-N3	4.10	120.54	114.80
2	K	500	UDX	N3-C2-N1	4.06	120.18	114.89
2	H	500	UDX	N3-C2-N1	4.06	120.17	114.89
2	K	501	UDX	C5-C4-N3	4.06	120.48	114.80
2	F	500	UDX	C5-C4-N3	4.03	120.45	114.80
2	A	501	UDX	C5-C4-N3	4.01	120.42	114.80
2	K	501	UDX	N3-C2-N1	4.00	120.10	114.89
2	J	500	UDX	N3-C2-N1	3.99	120.08	114.89
2	I	500	UDX	C5-C4-N3	3.97	120.37	114.80
2	B	501	UDX	C5-C4-N3	3.95	120.33	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	501	UDX	C5-C4-N3	3.95	120.33	114.80
2	G	500	UDX	N3-C2-N1	3.92	120.00	114.89
2	K	500	UDX	C5-C4-N3	3.92	120.29	114.80
2	G	501	UDX	C5-C4-N3	3.92	120.29	114.80
2	H	500	UDX	C5-C4-N3	3.92	120.29	114.80
2	G	500	UDX	C5-C4-N3	3.89	120.25	114.80
2	J	500	UDX	C5-C4-N3	3.86	120.21	114.80
2	L	500	UDX	C5-C4-N3	3.85	120.19	114.80
2	B	500	UDX	C5-C4-N3	3.82	120.16	114.80
2	H	501	UDX	C5-C4-N3	3.82	120.15	114.80
2	I	501	UDX	C5-C4-N3	3.79	120.11	114.80
2	C	500	UDX	C5-C4-N3	3.79	120.11	114.80
2	C	501	UDX	C5-C4-N3	3.79	120.11	114.80
2	D	500	UDX	C5-C4-N3	3.74	120.03	114.80
2	L	501	UDX	C5-C4-N3	3.73	120.03	114.80
2	E	501	UDX	C5-C4-N3	3.69	119.97	114.80
2	A	500	UDX	C5-C4-N3	3.68	119.95	114.80
2	H	501	UDX	N3-C2-N1	3.64	119.63	114.89
2	G	501	UDX	O2-C2-N1	-3.61	118.09	122.80
2	H	501	UDX	O4-C4-C5	-3.54	119.05	125.16
2	E	500	UDX	C5-C4-N3	3.53	119.75	114.80
2	A	501	UDX	O2-C2-N1	-3.26	118.55	122.80
2	K	500	UDX	O4-C4-C5	-3.26	119.55	125.16
2	E	500	UDX	O4-C4-C5	-3.24	119.57	125.16
2	I	501	UDX	O2-C2-N1	-3.17	118.67	122.80
2	G	500	UDX	O4-C4-C5	-3.06	119.88	125.16
2	G	501	UDX	O4-C4-C5	-3.03	119.94	125.16
2	L	500	UDX	O2-C2-N1	-3.02	118.87	122.80
2	B	500	UDX	O4-C4-C5	-3.00	119.99	125.16
2	D	500	UDX	O4-C4-C5	-2.99	120.01	125.16
2	F	501	UDX	O2-C2-N1	-2.98	118.91	122.80
2	B	501	UDX	O2-C2-N1	-2.97	118.92	122.80
2	J	500	UDX	O4-C4-C5	-2.97	120.05	125.16
2	L	500	UDX	O4-C4-C5	-2.96	120.05	125.16
2	H	500	UDX	O4-C4-C5	-2.95	120.08	125.16
2	I	500	UDX	O4-C4-C5	-2.92	120.13	125.16
2	E	501	UDX	O4-C4-C5	-2.91	120.15	125.16
2	A	500	UDX	O4-C4-C5	-2.89	120.17	125.16
2	K	500	UDX	O2-C2-N1	-2.82	119.13	122.80
2	C	500	UDX	O4-C4-C5	-2.82	120.30	125.16
2	A	500	UDX	O2-C2-N1	-2.80	119.16	122.80
2	A	501	UDX	O4-C4-C5	-2.78	120.37	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	500	UDX	O4-C4-C5	-2.77	120.39	125.16
2	E	501	UDX	O2-C2-N1	-2.76	119.20	122.80
2	H	501	UDX	O2-C2-N1	-2.73	119.24	122.80
2	E	500	UDX	O2-C2-N1	-2.71	119.27	122.80
2	J	501	UDX	O4-C4-C5	-2.71	120.49	125.16
2	L	501	UDX	O2-C2-N1	-2.69	119.29	122.80
2	C	501	UDX	O4-C4-C5	-2.69	120.52	125.16
2	I	501	UDX	O4-C4-C5	-2.69	120.53	125.16
2	I	501	UDX	O2A-PA-O3A	2.64	114.41	107.27
2	D	500	UDX	O2-C2-N1	-2.61	119.40	122.80
2	B	500	UDX	O2-C2-N1	-2.60	119.41	122.80
2	C	501	UDX	O2-C2-N1	-2.58	119.44	122.80
2	F	501	UDX	O4-C4-C5	-2.56	120.74	125.16
2	D	501	UDX	O4-C4-C5	-2.54	120.78	125.16
2	J	501	UDX	O2-C2-N1	-2.50	119.54	122.80
2	G	500	UDX	O2-C2-N1	-2.49	119.56	122.80
2	F	501	UDX	C5-C6-N1	-2.44	117.88	121.84
2	H	501	UDX	O2A-PA-O3A	2.44	113.86	107.27
2	B	501	UDX	O4-C4-C5	-2.42	120.98	125.16
2	K	501	UDX	O2-C2-N1	-2.40	119.67	122.80
2	I	500	UDX	O2-C2-N1	-2.37	119.71	122.80
2	K	501	UDX	O2A-PA-O3A	2.33	113.57	107.27
2	K	501	UDX	O4-C4-C5	-2.33	121.15	125.16
2	L	501	UDX	O2A-PA-O3A	2.32	113.55	107.27
2	L	501	UDX	O4-C4-C5	-2.28	121.23	125.16
2	C	501	UDX	O2A-PA-O3A	2.23	113.31	107.27
2	B	500	UDX	O4D-C1D-N1	2.19	113.33	108.36
2	D	500	UDX	O4D-C1D-N1	2.19	113.32	108.36
2	F	501	UDX	O2A-PA-O3A	2.16	113.12	107.27
2	G	501	UDX	C5-C6-N1	-2.16	118.32	121.84
2	D	501	UDX	O2-C2-N1	-2.12	120.03	122.80
2	A	501	UDX	O3D-C3D-C4D	-2.09	105.07	111.08
2	K	501	UDX	O3D-C3D-C4D	-2.06	105.16	111.08
2	B	501	UDX	C5-C6-N1	-2.05	118.51	121.84
2	E	500	UDX	O4D-C1D-N1	2.02	112.94	108.36
2	H	500	UDX	O2-C2-N1	-2.01	120.18	122.80

There are no chirality outliers.

All (121) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	UDX	C1'-O3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	A	501	UDX	C1'-O3B-PB-O3A
2	A	501	UDX	PA-O3A-PB-O3B
2	B	501	UDX	C1'-O3B-PB-O1B
2	B	501	UDX	C1'-O3B-PB-O3A
2	B	501	UDX	C5D-O5D-PA-O2A
2	C	500	UDX	C1'-O3B-PB-O2B
2	C	501	UDX	PA-O3A-PB-O3B
2	D	500	UDX	C1'-O3B-PB-O2B
2	D	501	UDX	C1'-O3B-PB-O3A
2	D	501	UDX	PA-O3A-PB-O3B
2	E	500	UDX	C1'-O3B-PB-O2B
2	E	500	UDX	C1'-O3B-PB-O3A
2	E	501	UDX	C1'-O3B-PB-O3A
2	F	500	UDX	C1'-O3B-PB-O2B
2	F	501	UDX	C1'-O3B-PB-O1B
2	F	501	UDX	C1'-O3B-PB-O3A
2	F	501	UDX	C5D-O5D-PA-O3A
2	F	501	UDX	C5D-O5D-PA-O2A
2	G	501	UDX	C1'-O3B-PB-O1B
2	G	501	UDX	C1'-O3B-PB-O3A
2	J	500	UDX	C1'-O3B-PB-O2B
2	J	500	UDX	C1'-O3B-PB-O3A
2	J	501	UDX	C1'-O3B-PB-O1B
2	J	501	UDX	C1'-O3B-PB-O3A
2	J	501	UDX	PA-O3A-PB-O3B
2	K	500	UDX	C1'-O3B-PB-O2B
2	L	501	UDX	C1'-O3B-PB-O3A
2	L	501	UDX	PA-O3A-PB-O3B
2	F	501	UDX	O4D-C4D-C5D-O5D
2	F	501	UDX	C3D-C4D-C5D-O5D
2	B	500	UDX	C2'-C1'-O3B-PB
2	C	500	UDX	C2'-C1'-O3B-PB
2	F	500	UDX	C2'-C1'-O3B-PB
2	G	500	UDX	C2'-C1'-O3B-PB
2	H	500	UDX	C2'-C1'-O3B-PB
2	L	500	UDX	C2'-C1'-O3B-PB
2	K	500	UDX	O4D-C4D-C5D-O5D
2	K	500	UDX	C3D-C4D-C5D-O5D
2	A	500	UDX	C2'-C1'-O3B-PB
2	D	500	UDX	C2'-C1'-O3B-PB
2	I	500	UDX	C2'-C1'-O3B-PB
2	K	500	UDX	C2'-C1'-O3B-PB

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

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Mol	Chain	Res	Type	Atoms
2	J	501	UDX	PB-O3A-PA-O2A
2	K	501	UDX	PB-O3A-PA-O2A
2	L	501	UDX	PB-O3A-PA-O2A
2	I	500	UDX	O4D-C4D-C5D-O5D
2	C	500	UDX	O4D-C4D-C5D-O5D
2	H	500	UDX	C3D-C4D-C5D-O5D
2	D	501	UDX	PB-O3A-PA-O1A
2	D	501	UDX	PB-O3A-PA-O2A
2	B	500	UDX	O4D-C1D-N1-C6
2	A	500	UDX	C1'-O3B-PB-O1B
2	B	500	UDX	C1'-O3B-PB-O1B
2	C	500	UDX	C1'-O3B-PB-O1B
2	D	500	UDX	C1'-O3B-PB-O1B
2	G	500	UDX	C1'-O3B-PB-O1B
2	H	500	UDX	C1'-O3B-PB-O1B
2	I	500	UDX	C1'-O3B-PB-O1B
2	J	500	UDX	C1'-O3B-PB-O1B
2	K	500	UDX	C1'-O3B-PB-O1B
2	L	500	UDX	C1'-O3B-PB-O1B
2	B	500	UDX	C2D-C1D-N1-C6
2	D	500	UDX	O4D-C4D-C5D-O5D
2	G	500	UDX	O4D-C4D-C5D-O5D
2	B	501	UDX	PB-O3A-PA-O2A
2	F	501	UDX	PB-O3A-PA-O1A
2	F	501	UDX	PB-O3A-PA-O2A
2	G	501	UDX	PB-O3A-PA-O2A
2	I	501	UDX	PB-O3A-PA-O1A
2	K	501	UDX	PB-O3A-PA-O1A
2	H	501	UDX	C2'-C1'-O3B-PB
2	K	501	UDX	C2'-C1'-O3B-PB
2	E	500	UDX	PB-O3A-PA-O2A
2	E	501	UDX	PB-O3A-PA-O2A
2	J	500	UDX	PB-O3A-PA-O2A
2	F	500	UDX	O4D-C4D-C5D-O5D
2	J	501	UDX	O4D-C4D-C5D-O5D
2	J	501	UDX	C3D-C4D-C5D-O5D

There are no ring outliers.

8 monomers are involved in 8 short contacts:

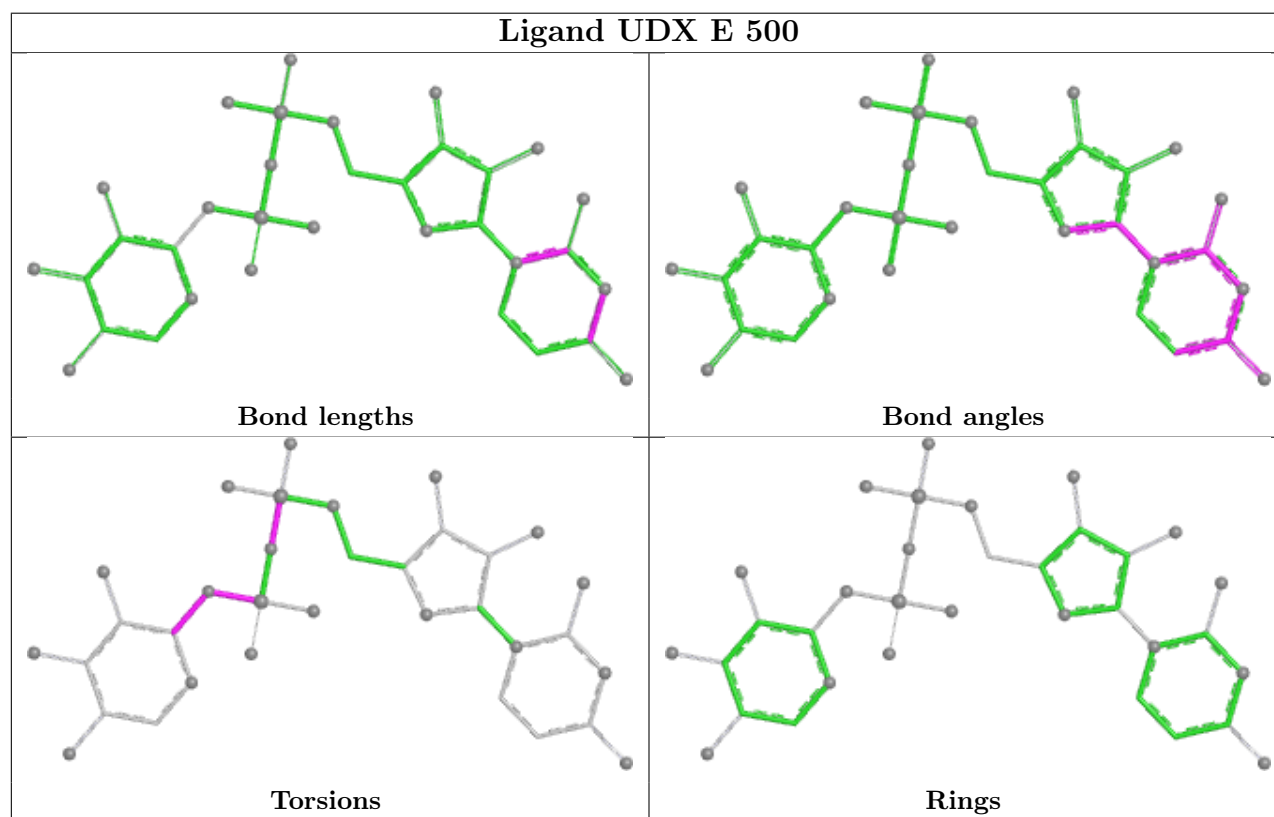
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	500	UDX	1	0

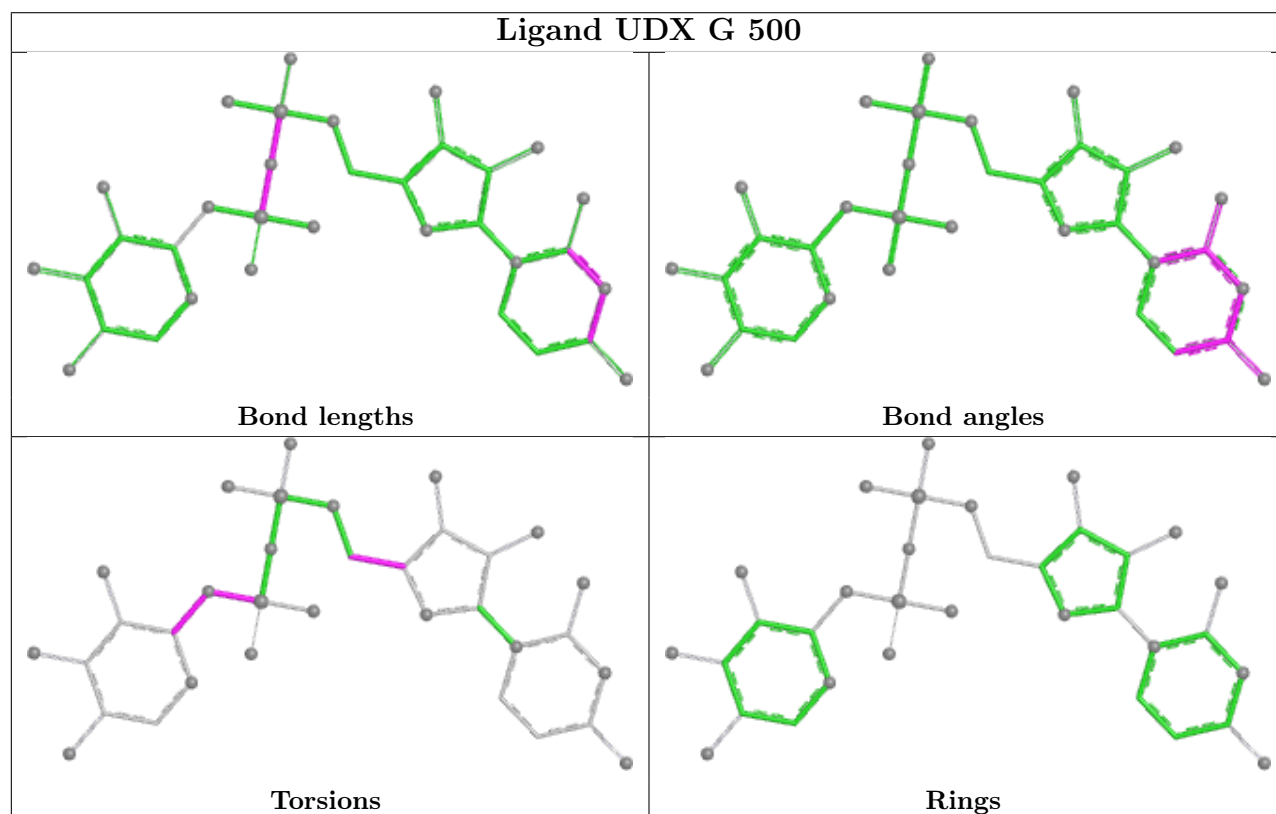
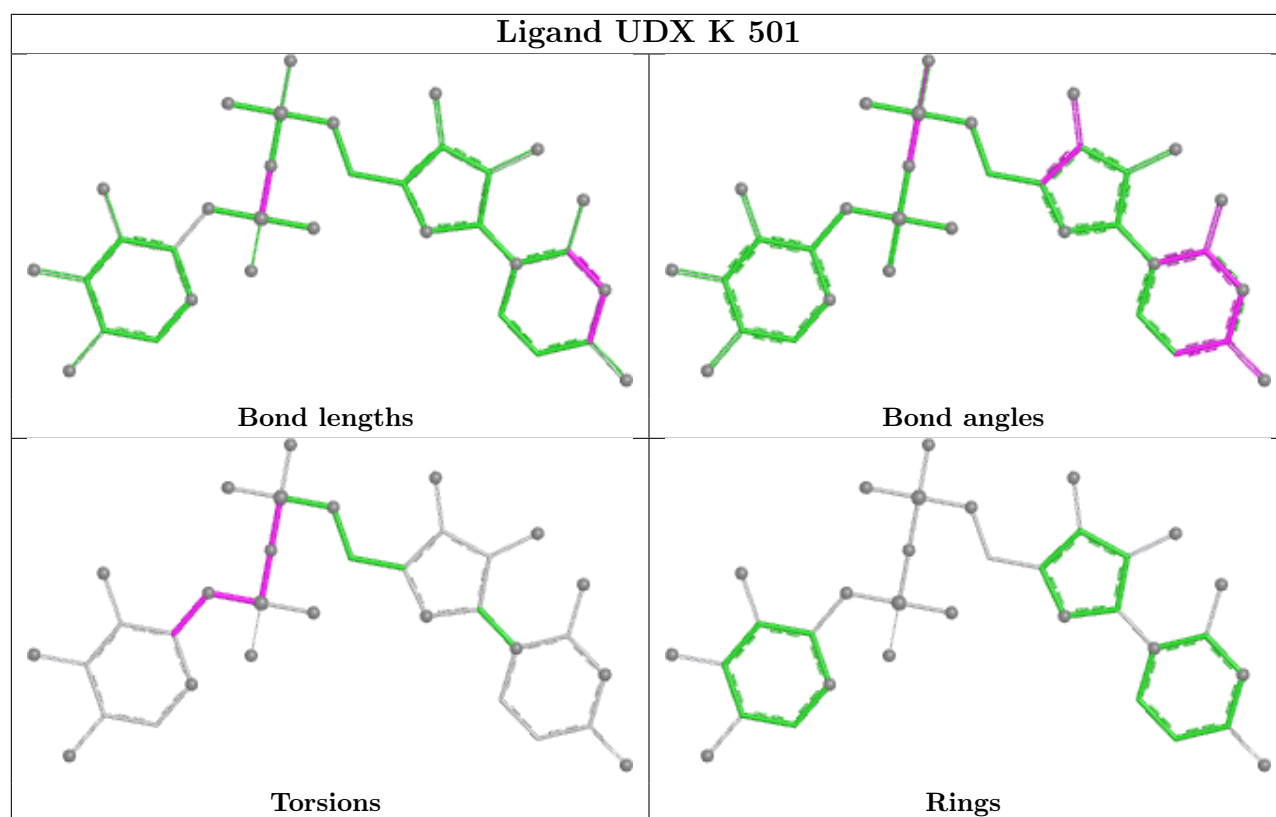
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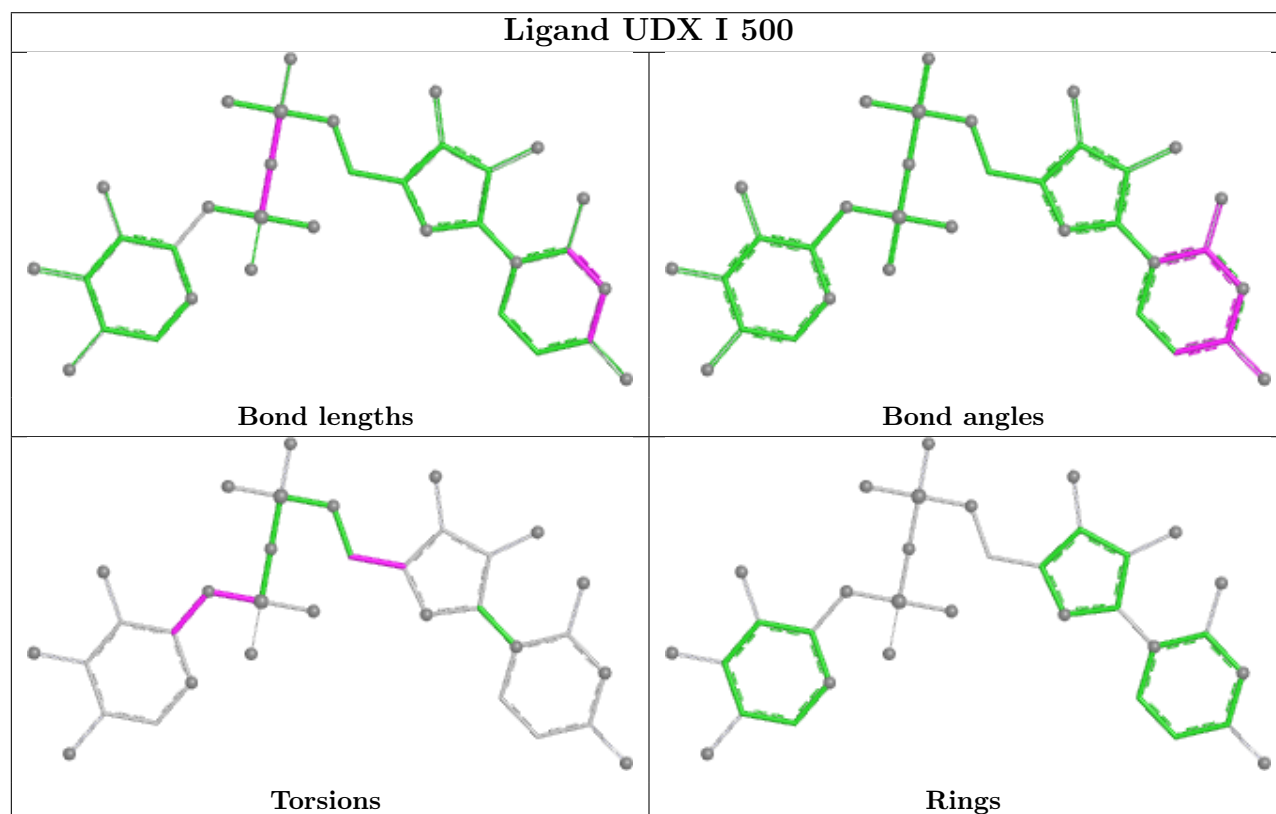
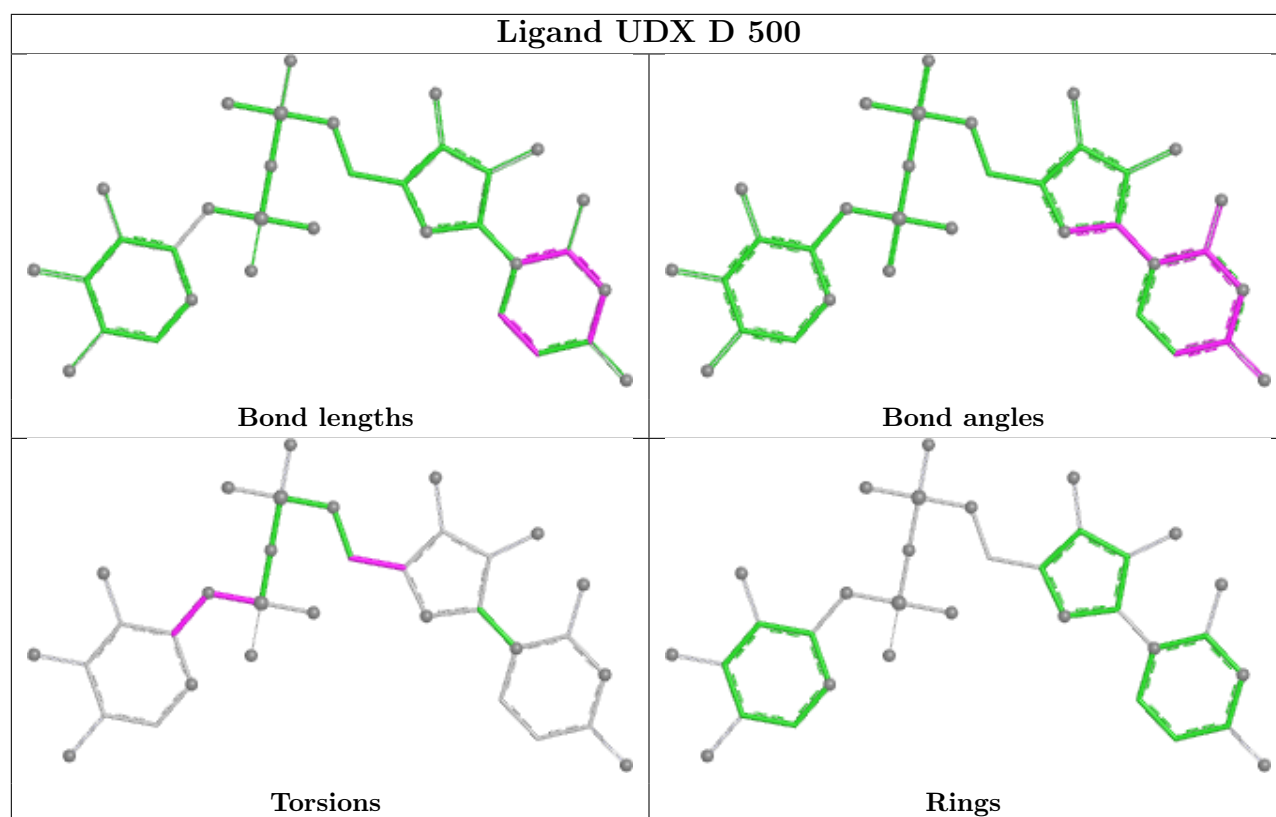
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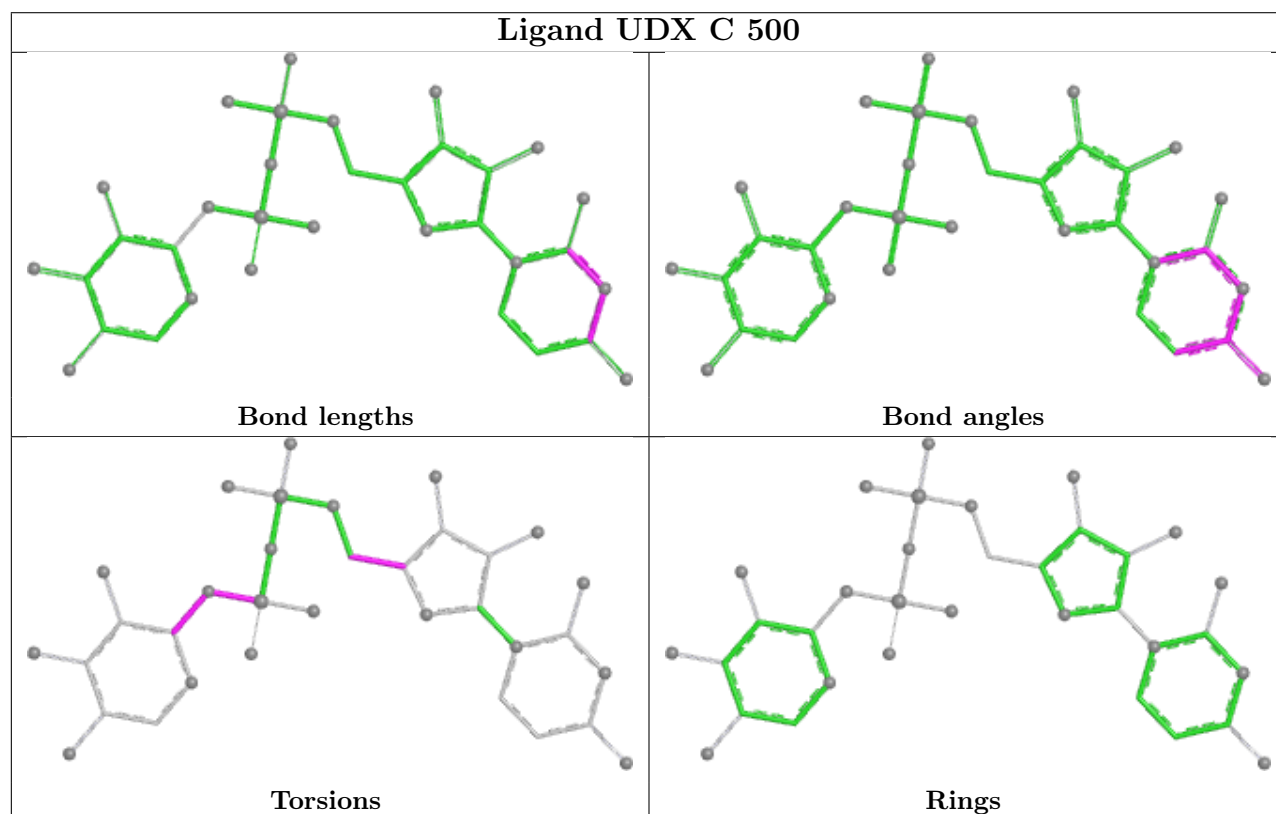
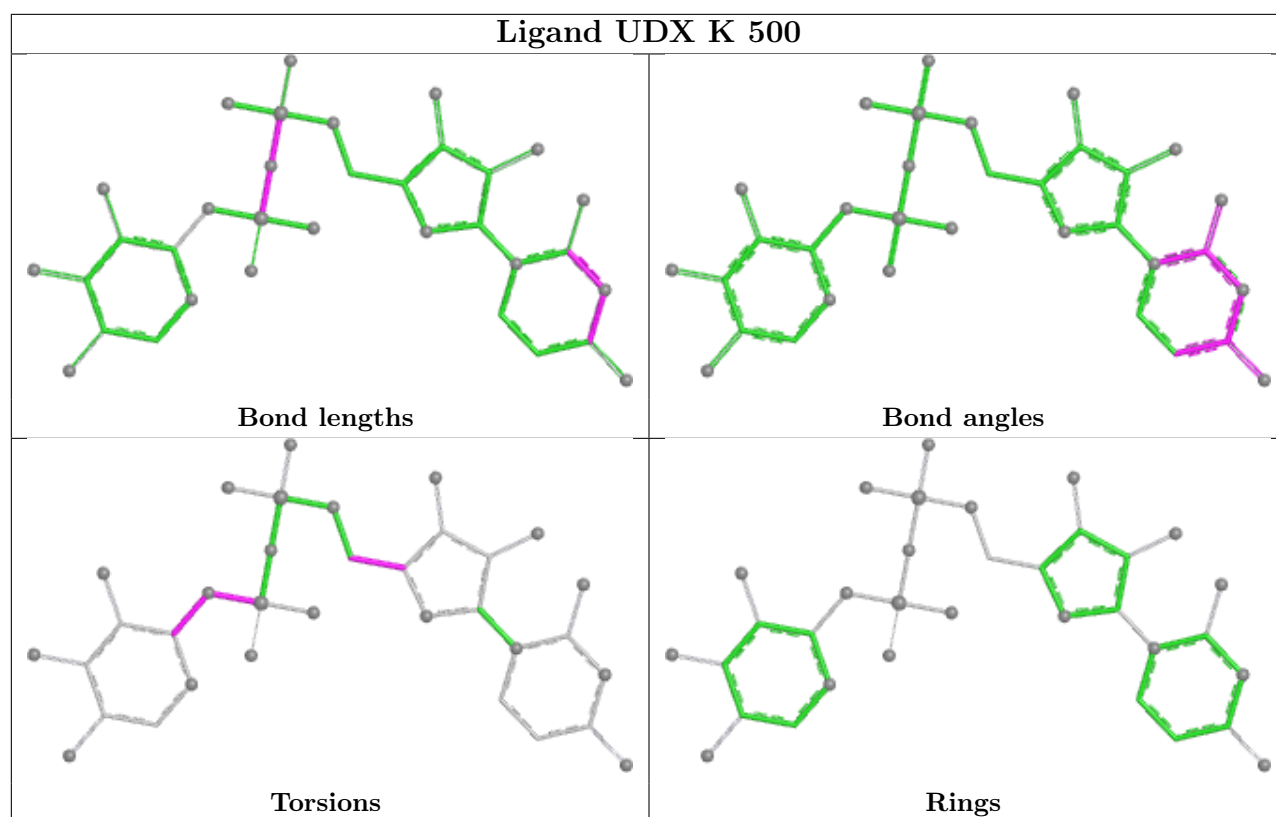
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	500	UDX	1	0
2	D	500	UDX	1	0
2	I	500	UDX	1	0
2	C	500	UDX	1	0
2	F	500	UDX	1	0
2	D	501	UDX	1	0
2	J	500	UDX	1	0

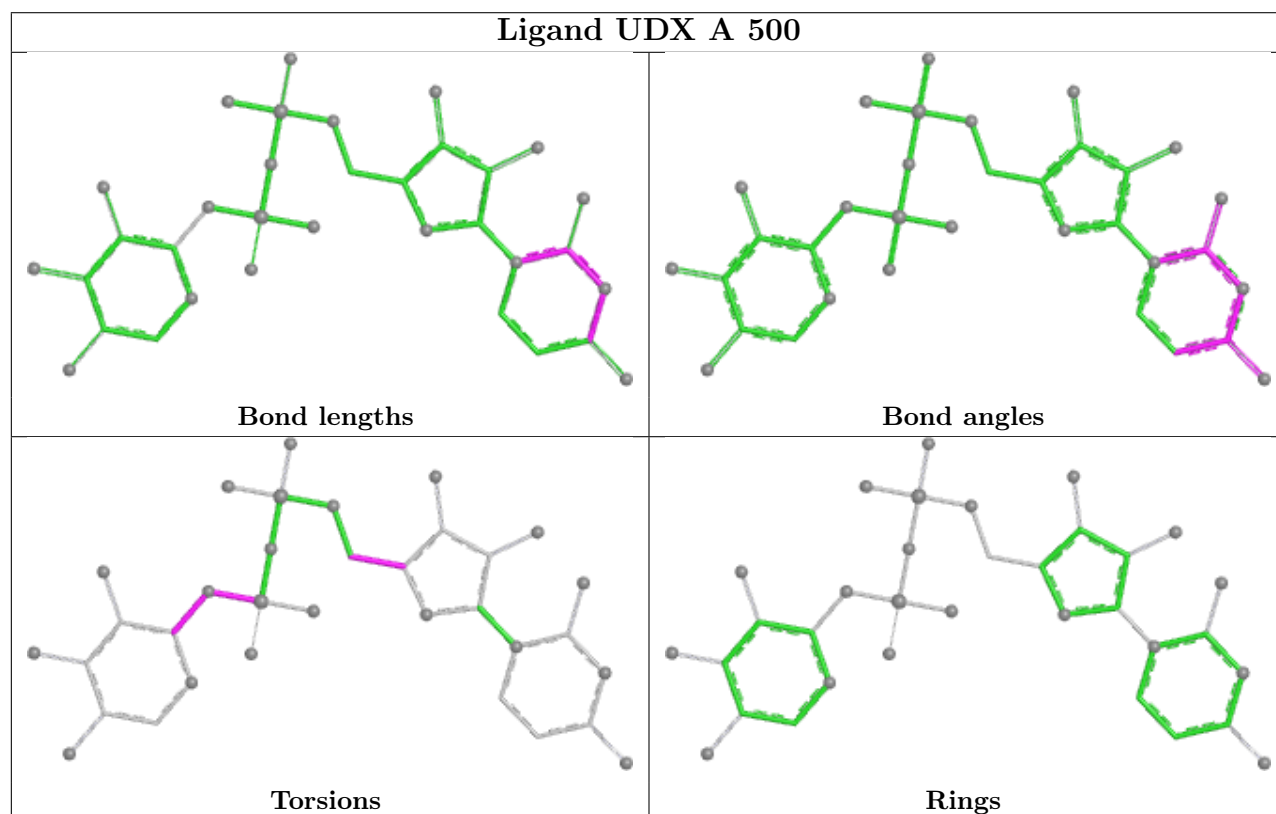
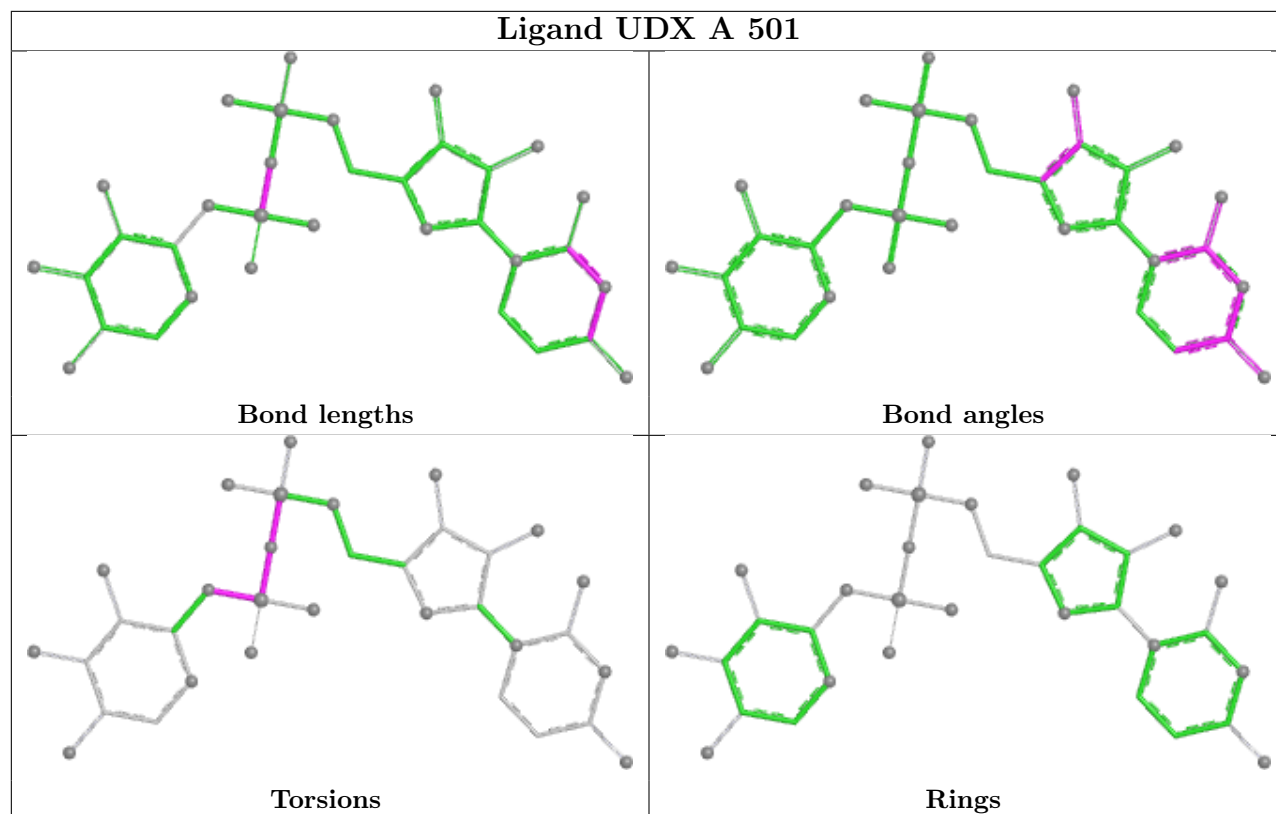
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

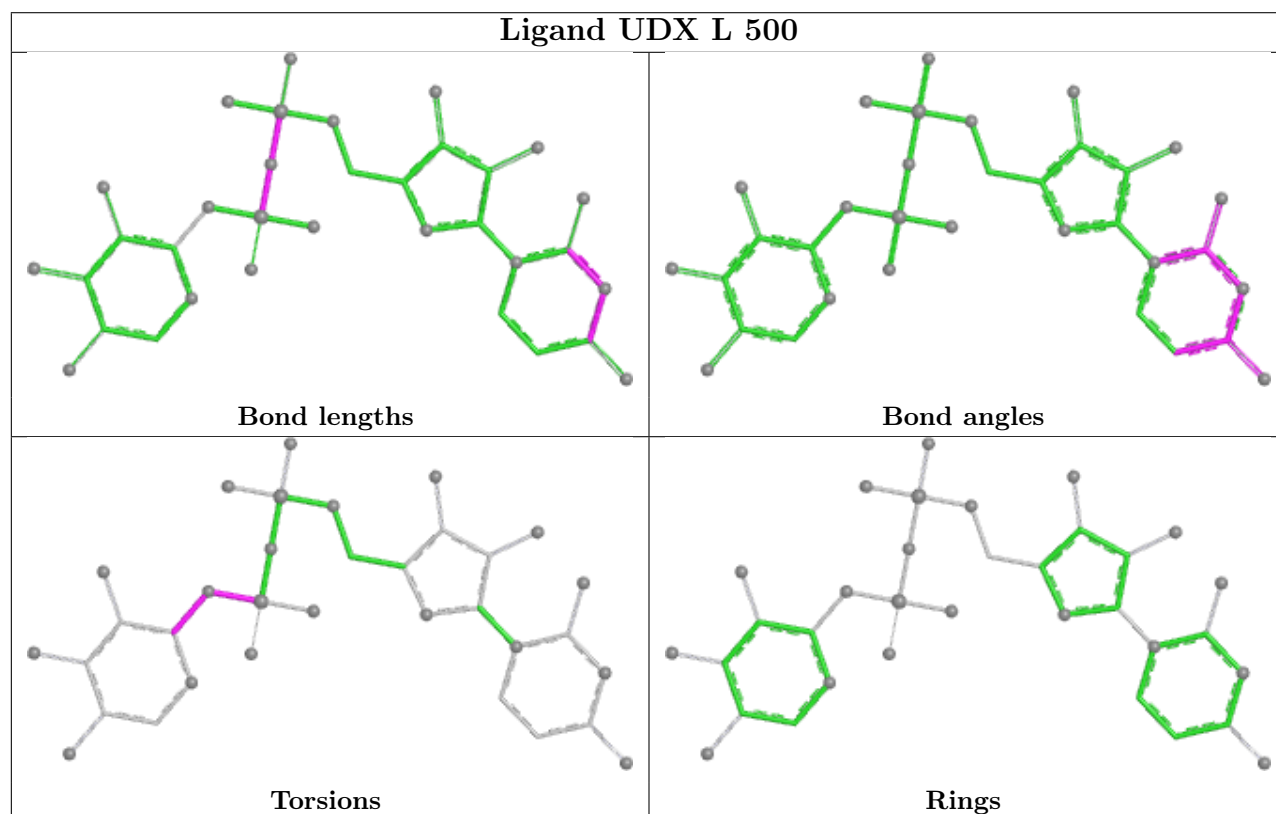
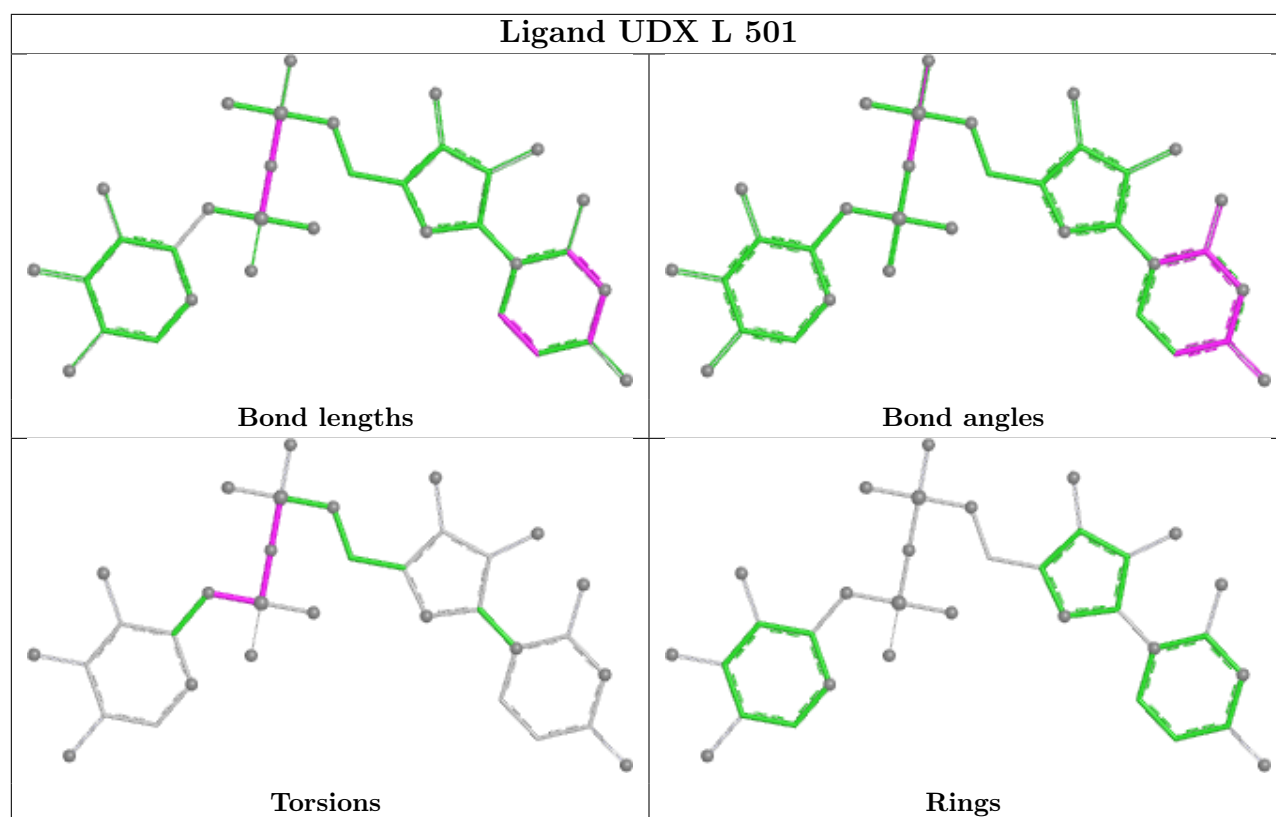


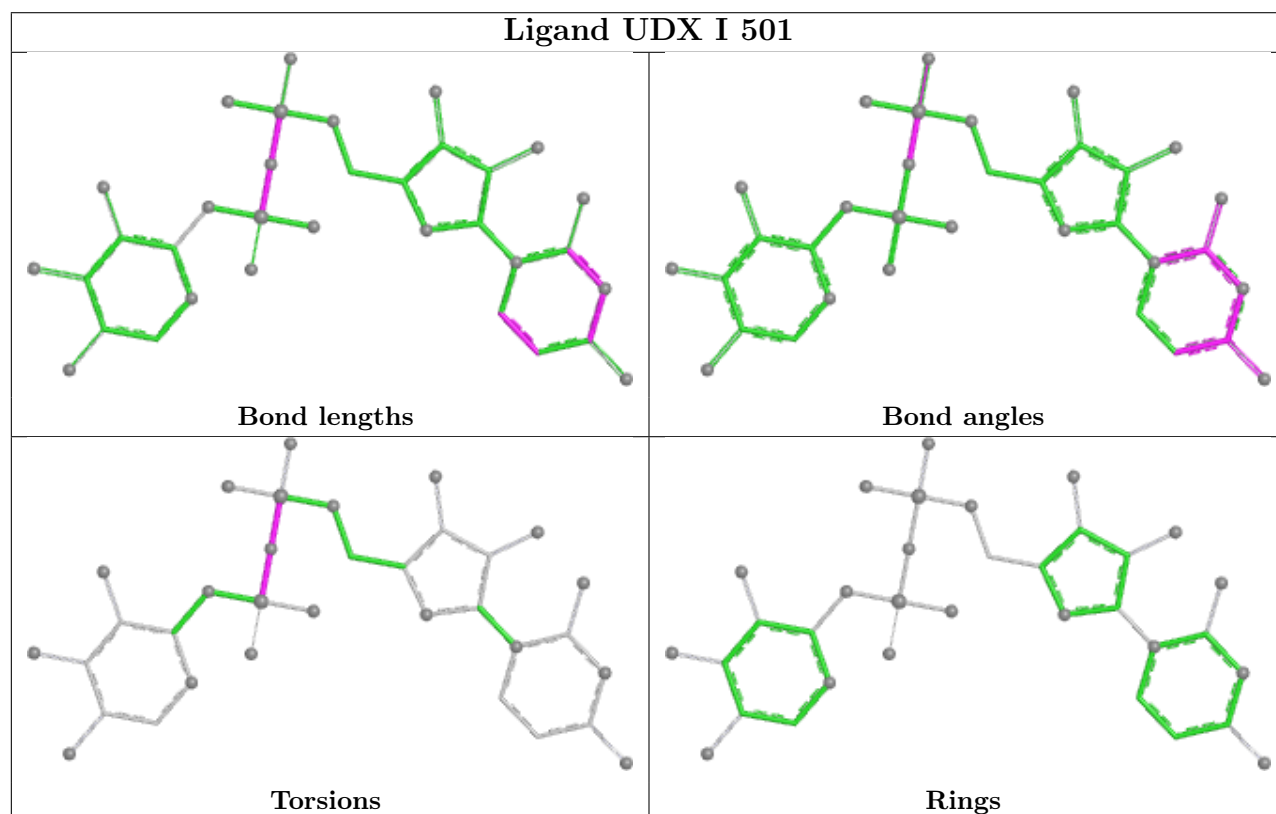
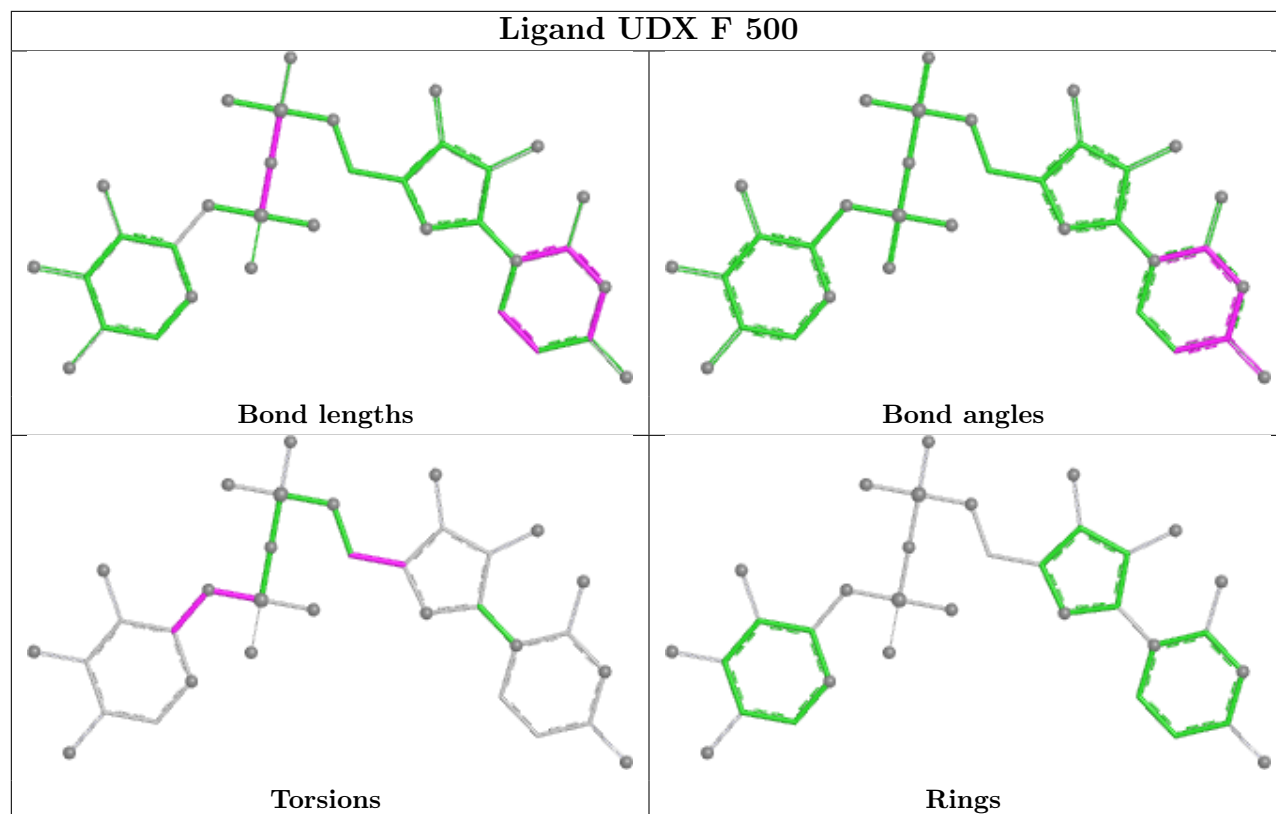


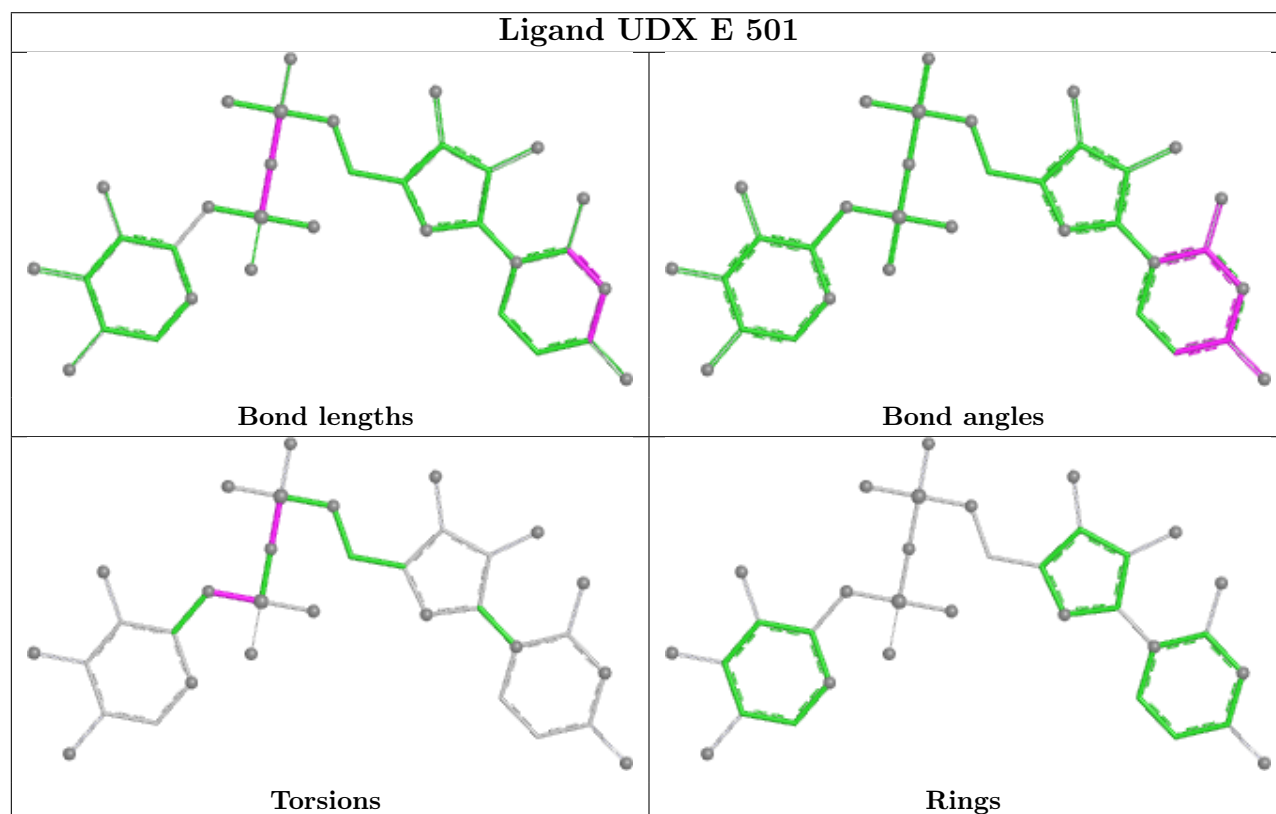
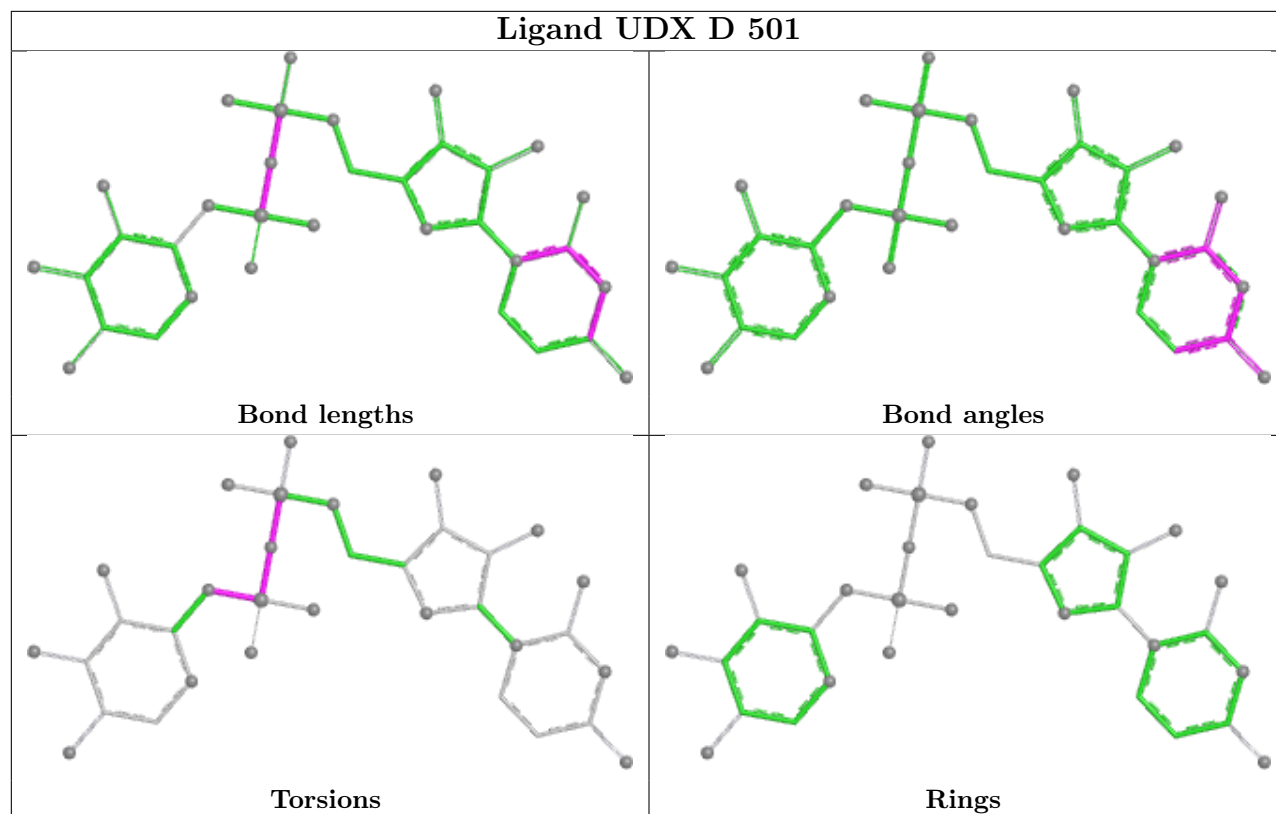


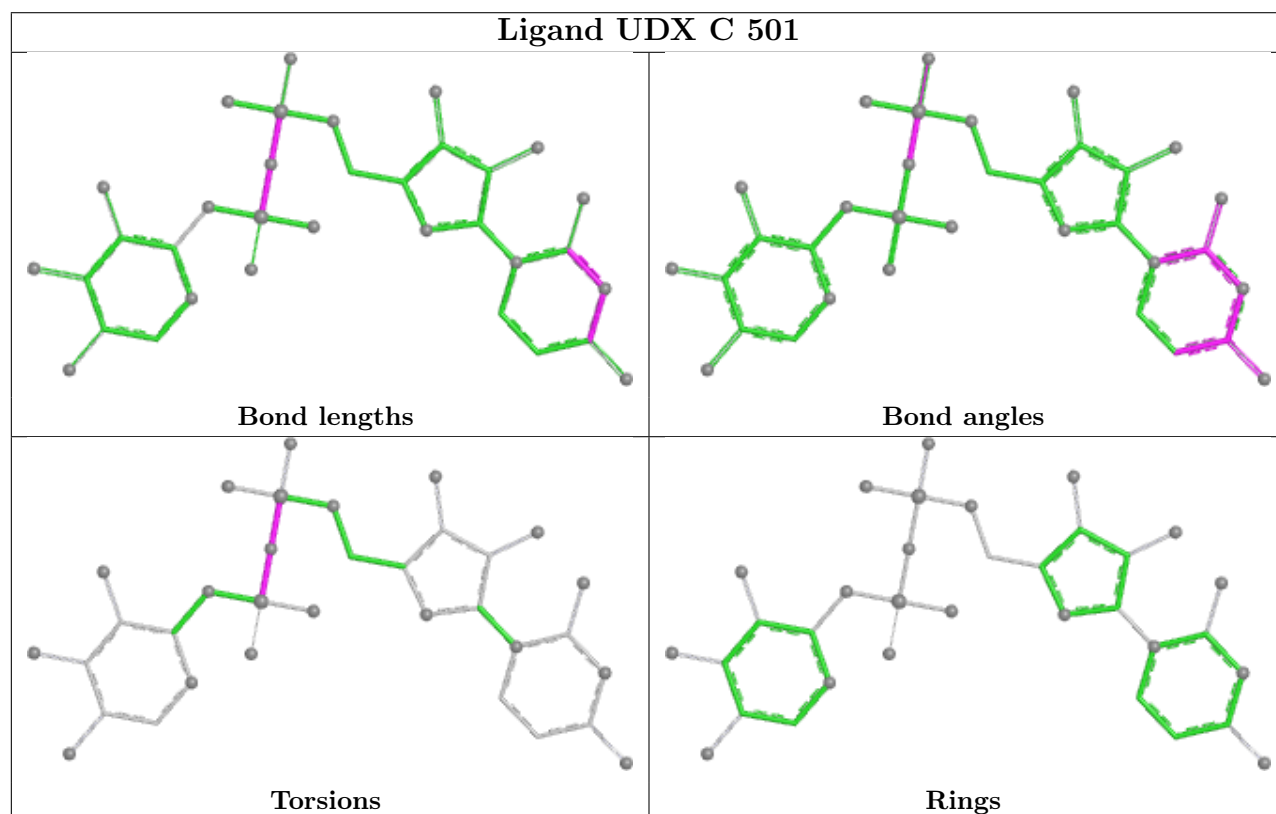
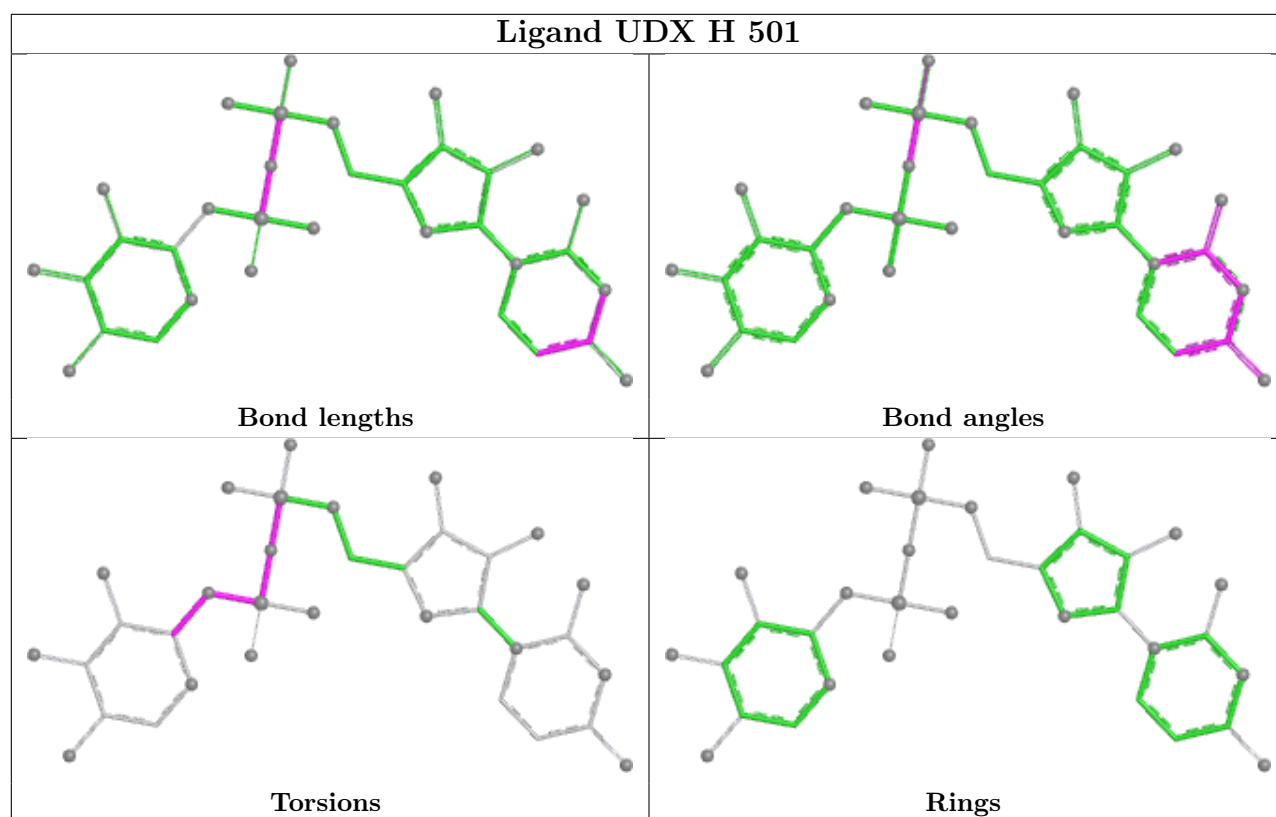


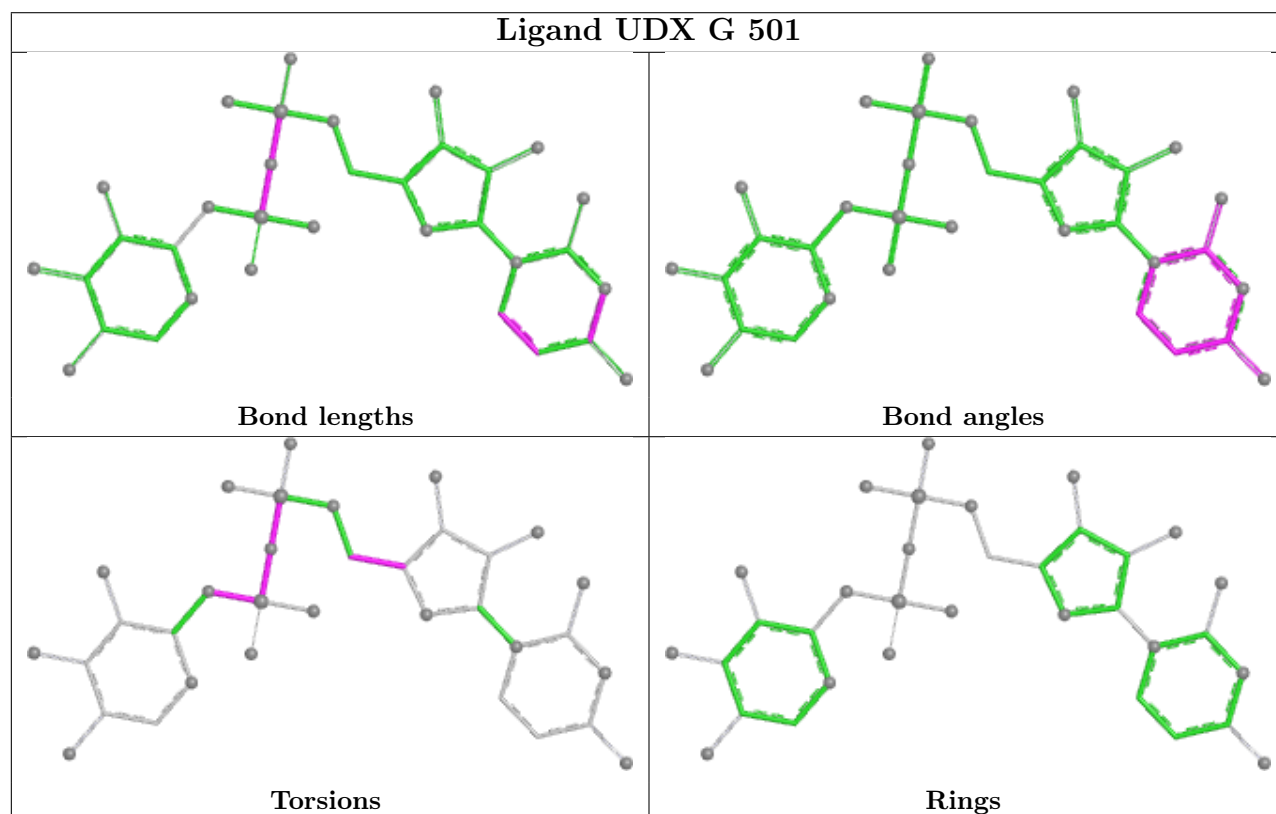
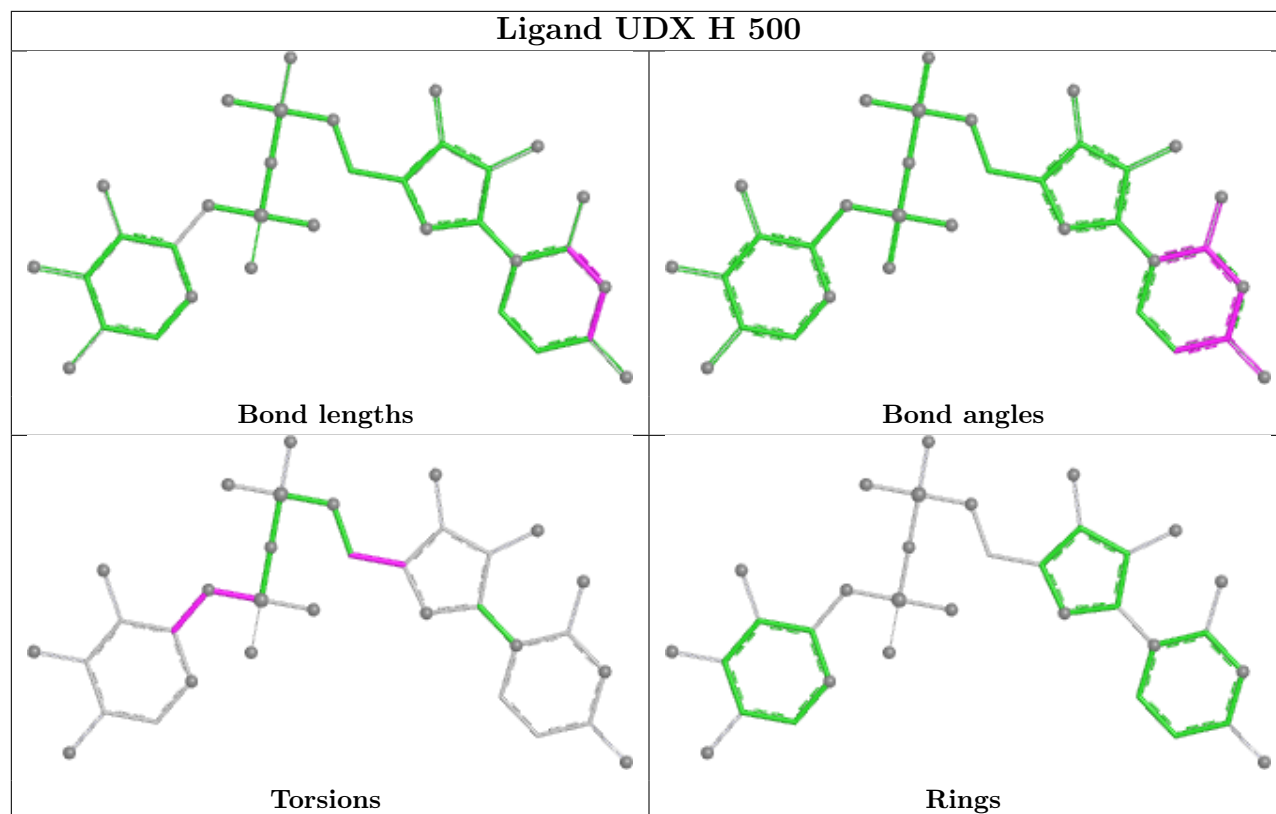


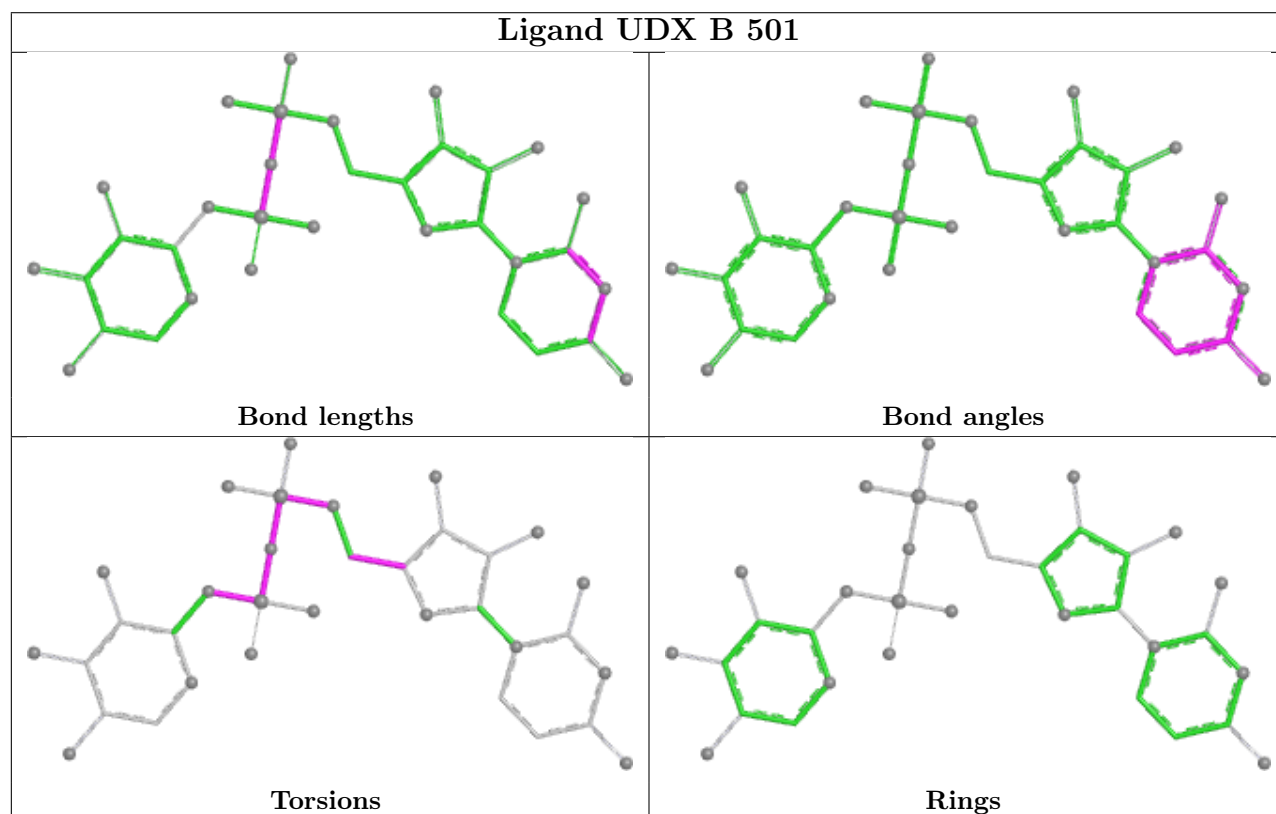
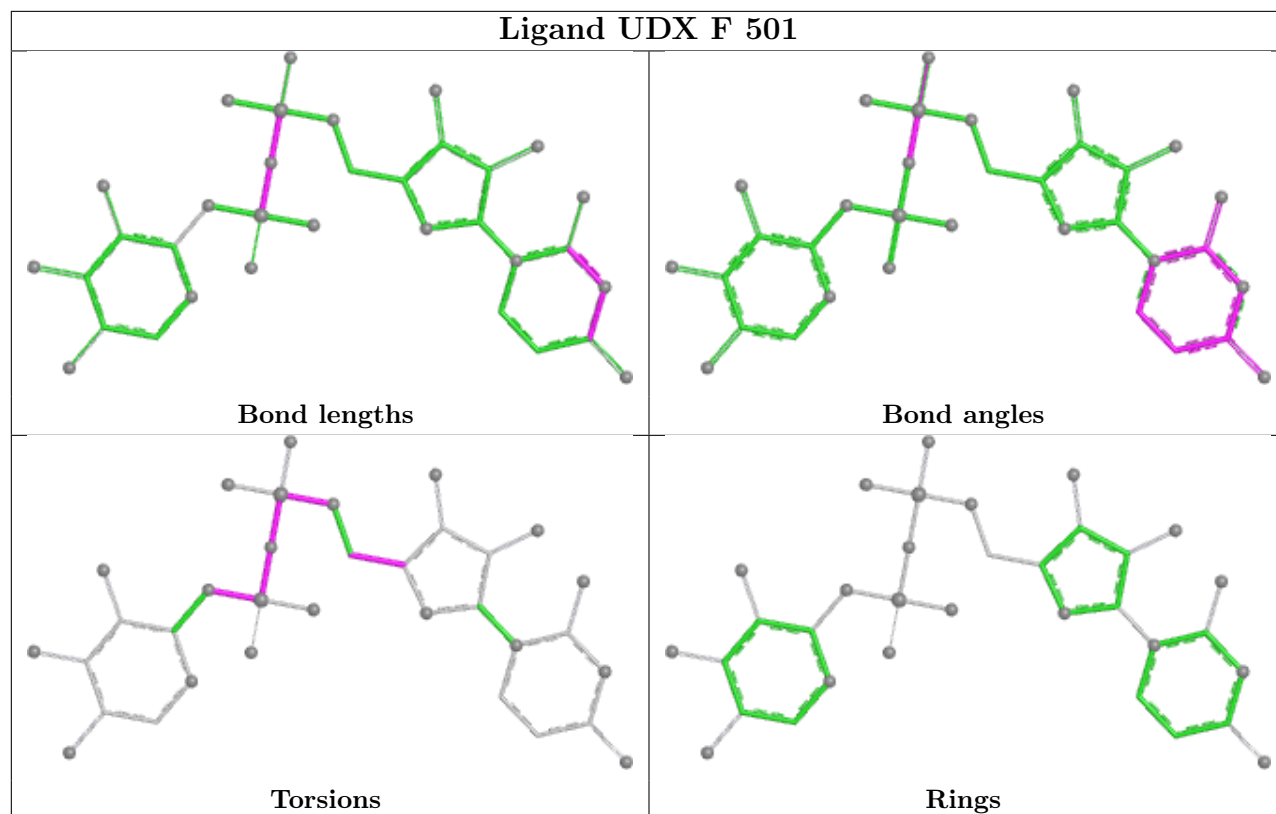


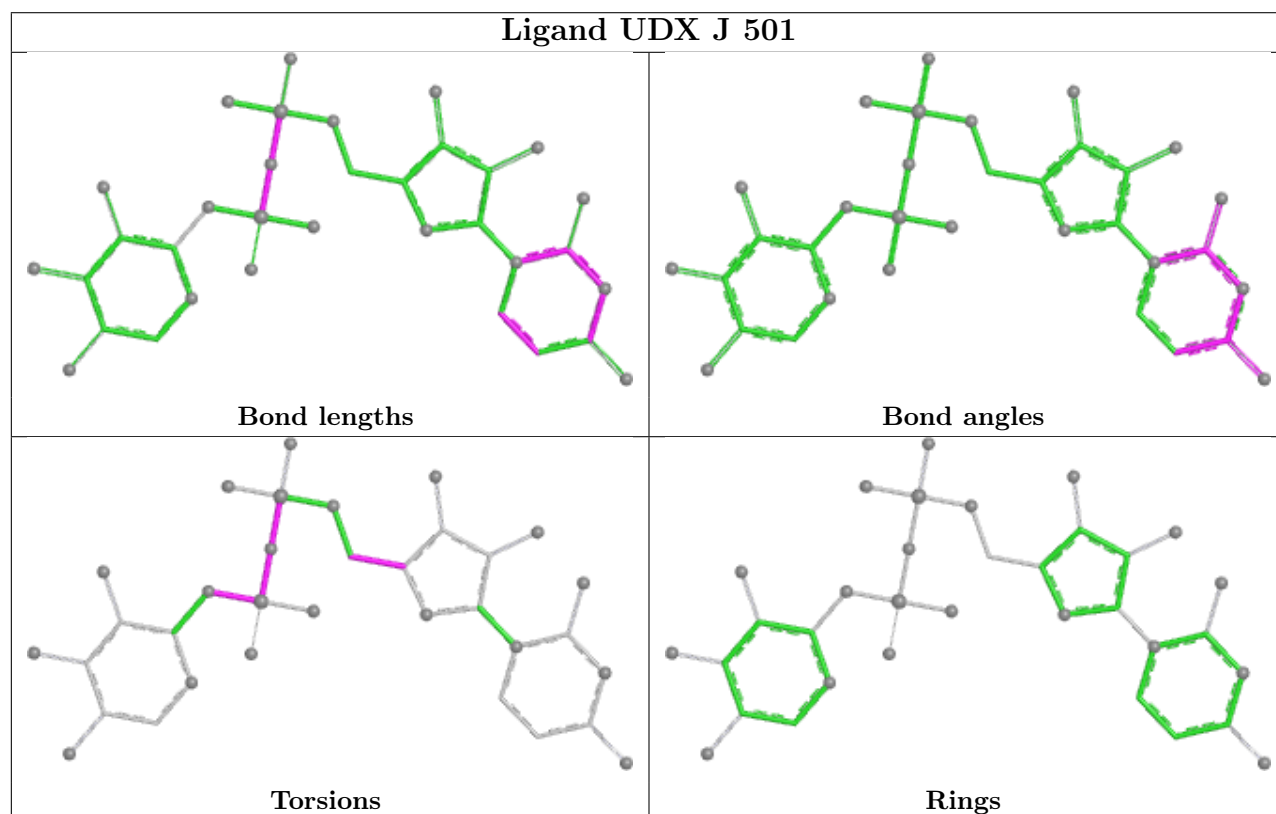
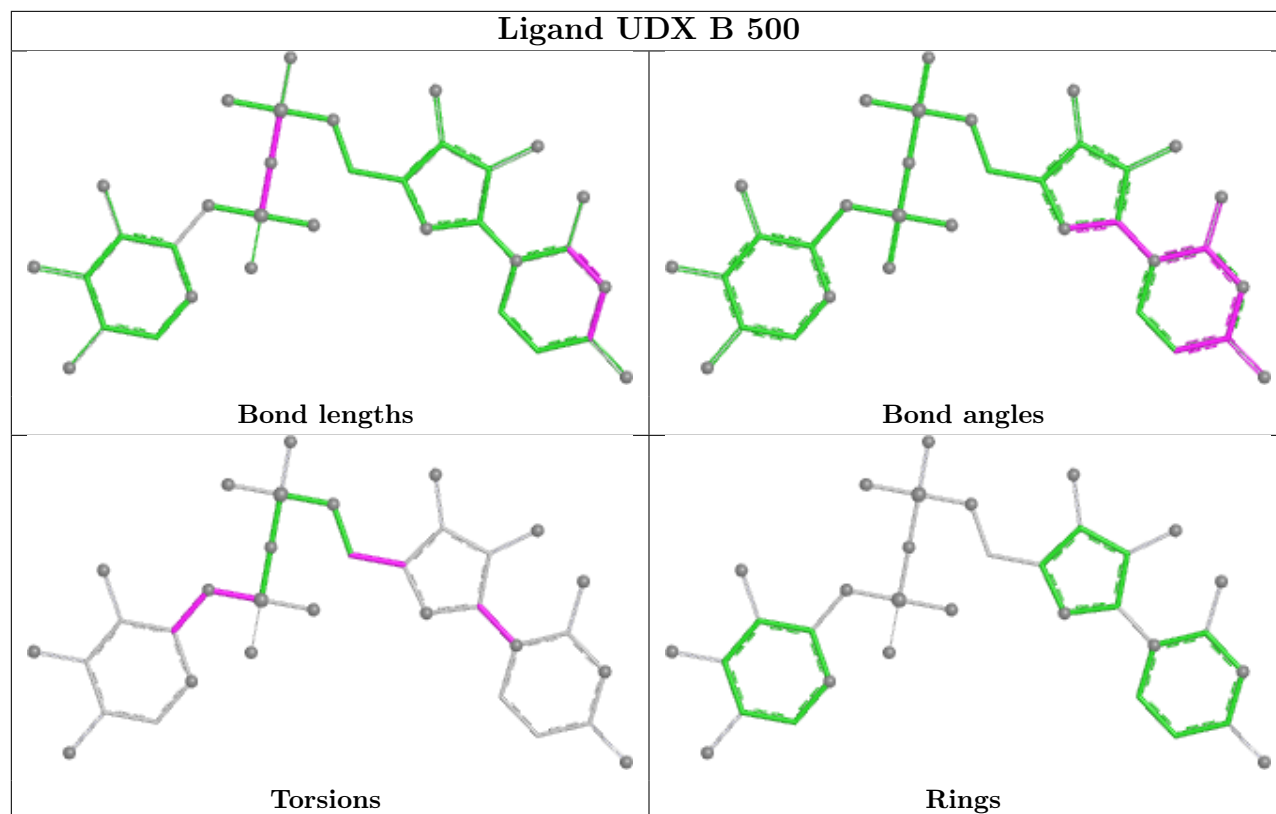


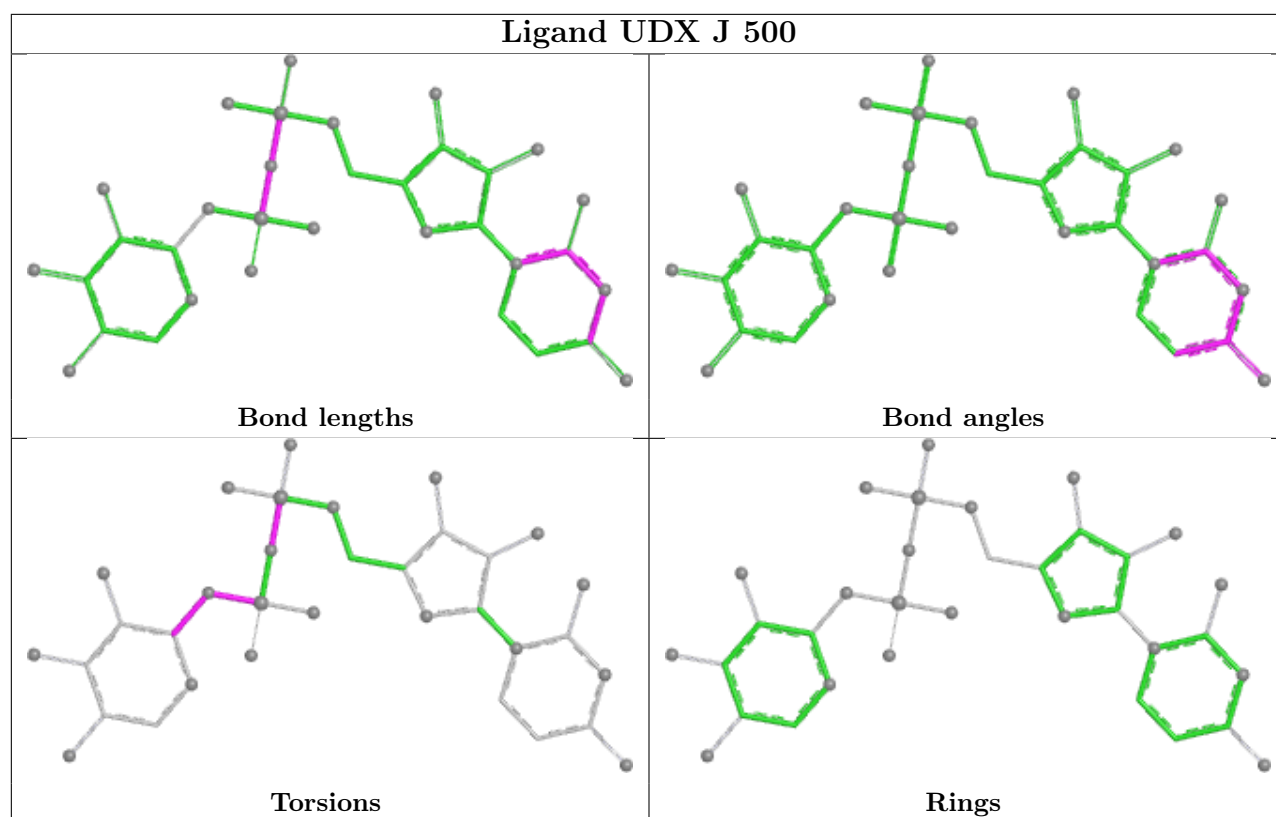












5.7 Other polymers [i](#)

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	463/481 (96%)	-0.17	1 (0%) 91 92	30, 43, 63, 101	0
1	B	463/481 (96%)	0.27	10 (2%) 62 63	24, 54, 83, 109	1 (0%)
1	C	463/481 (96%)	-0.03	4 (0%) 81 82	29, 48, 70, 97	1 (0%)
1	D	468/481 (97%)	-0.13	5 (1%) 78 79	28, 45, 69, 124	1 (0%)
1	E	461/481 (95%)	-0.10	5 (1%) 78 79	29, 45, 69, 107	2 (0%)
1	F	465/481 (96%)	-0.06	2 (0%) 88 90	23, 46, 67, 91	3 (0%)
1	G	462/481 (96%)	0.20	2 (0%) 88 90	31, 56, 77, 97	2 (0%)
1	H	462/481 (96%)	0.02	1 (0%) 91 92	24, 50, 72, 92	3 (0%)
1	I	462/481 (96%)	0.18	3 (0%) 85 87	33, 56, 77, 109	2 (0%)
1	J	456/481 (94%)	0.32	9 (1%) 65 66	35, 59, 86, 111	1 (0%)
1	K	464/481 (96%)	0.16	6 (1%) 75 77	25, 52, 78, 99	2 (0%)
1	L	463/481 (96%)	0.15	7 (1%) 72 73	33, 54, 78, 116	2 (0%)
All	All	5552/5772 (96%)	0.07	55 (0%) 79 81	23, 51, 76, 124	20 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	139	VAL	5.2
1	J	1	MET	5.0
1	E	100	MET	4.0
1	C	331	ASN	3.3
1	L	138	PRO	3.3
1	F	7	GLY	3.3
1	C	324	LYS	3.2
1	D	101	TYR	2.9
1	L	169	PHE	2.9
1	L	95	ASN	2.9
1	B	213	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	155	ASN	2.8
1	K	78	SER	2.7
1	H	139	VAL	2.7
1	E	139	VAL	2.7
1	G	101	TYR	2.7
1	G	139	VAL	2.6
1	K	139	VAL	2.6
1	E	160	LYS	2.6
1	E	103	ARG	2.5
1	B	100	MET	2.5
1	J	469	PRO	2.5
1	B	88	ASP	2.5
1	J	169	PHE	2.5
1	D	100	MET	2.5
1	B	9	VAL	2.4
1	C	104	GLY	2.4
1	L	102	GLY	2.4
1	L	101	TYR	2.4
1	D	139	VAL	2.4
1	J	154	LYS	2.4
1	K	359	HIS	2.4
1	I	333	VAL	2.4
1	F	470	ASP	2.4
1	A	139	VAL	2.4
1	B	33	PRO	2.3
1	D	379	GLN	2.3
1	J	98	THR	2.3
1	I	144	SER	2.3
1	E	95	ASN	2.3
1	B	126	GLY	2.3
1	B	197	GLN	2.3
1	B	69	ALA	2.2
1	C	78	SER	2.2
1	B	139	VAL	2.2
1	J	152	ALA	2.2
1	K	154	LYS	2.2
1	B	101	TYR	2.2
1	I	120	THR	2.2
1	L	100	MET	2.1
1	J	126	GLY	2.1
1	D	299	ASN	2.1
1	J	158	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	86	GLU	2.0
1	K	212	ARG	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 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	J	500	34/34	0.88	0.12	77,91,99,102	0
2	UDX	G	500	34/34	0.95	0.07	50,58,66,67	0
2	UDX	E	500	34/34	0.95	0.07	42,58,68,69	0
2	UDX	L	500	34/34	0.95	0.07	49,59,76,77	0
2	UDX	K	500	34/34	0.96	0.08	43,54,66,66	0
2	UDX	I	500	34/34	0.96	0.07	41,49,61,61	0
2	UDX	F	500	34/34	0.97	0.06	33,49,54,61	0
2	UDX	B	500	34/34	0.97	0.06	51,58,63,65	0
2	UDX	H	500	34/34	0.97	0.07	46,54,62,67	0
2	UDX	H	501	34/34	0.97	0.06	35,41,48,55	0
2	UDX	B	501	34/34	0.97	0.07	34,45,51,56	0
2	UDX	I	501	34/34	0.97	0.07	38,45,51,52	0
2	UDX	D	500	34/34	0.97	0.06	35,47,67,71	0
2	UDX	J	501	34/34	0.97	0.07	40,50,58,60	0
2	UDX	A	500	34/34	0.97	0.06	35,41,50,53	0
2	UDX	E	501	34/34	0.97	0.06	30,37,42,44	0
2	UDX	L	501	34/34	0.97	0.06	35,43,45,48	0
2	UDX	F	501	34/34	0.98	0.05	29,36,39,47	0
2	UDX	D	501	34/34	0.98	0.05	29,37,45,50	0
2	UDX	G	501	34/34	0.98	0.05	33,41,49,51	0
2	UDX	C	500	34/34	0.98	0.06	38,50,54,55	0

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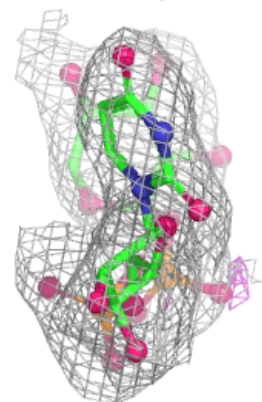
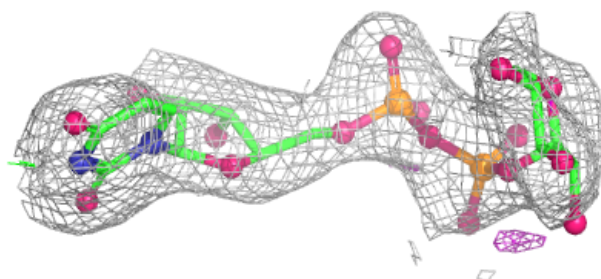
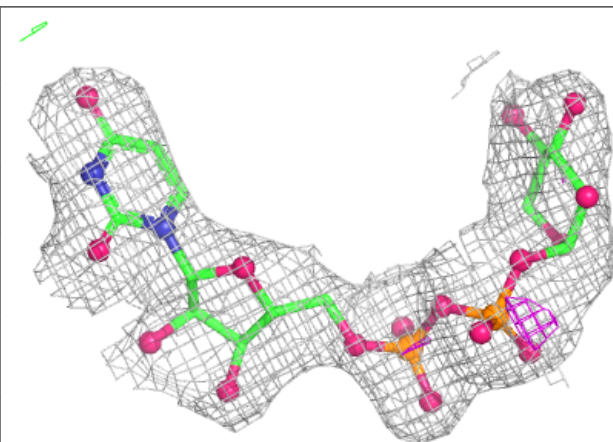
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UDX	K	501	34/34	0.98	0.05	30,40,45,47	0
2	UDX	C	501	34/34	0.98	0.06	29,36,42,43	0
2	UDX	A	501	34/34	0.98	0.05	28,37,42,45	0

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.

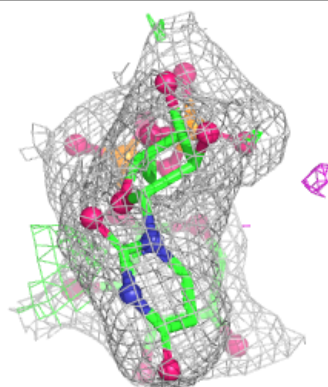
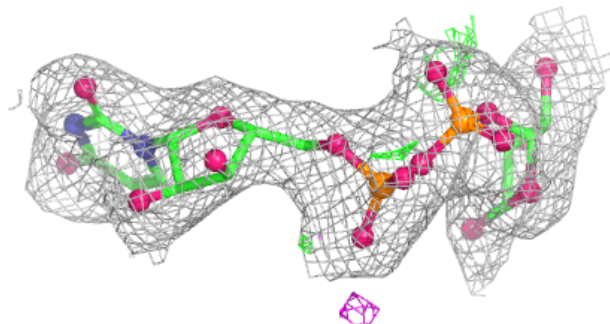
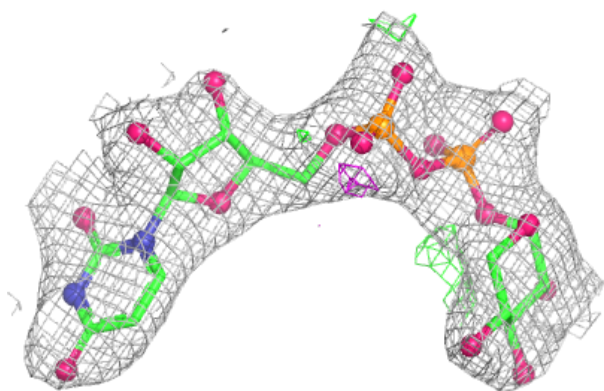
Electron density around UDX J 500:

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

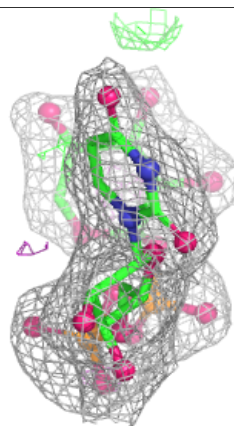
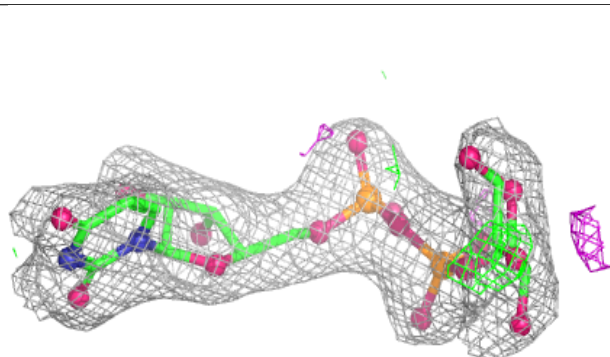
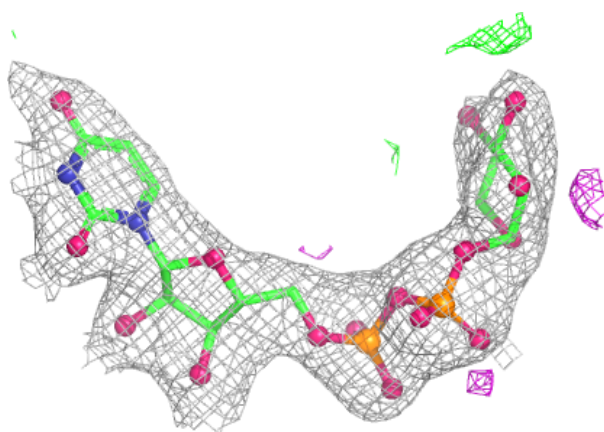


Electron density around UDX G 500:

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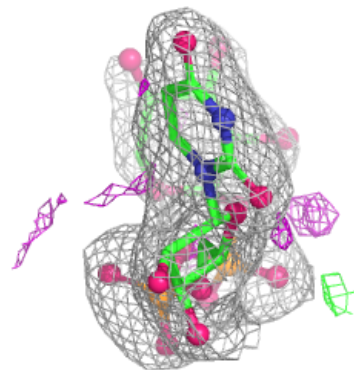
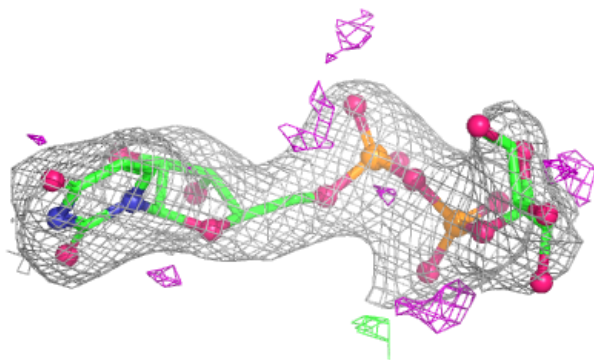
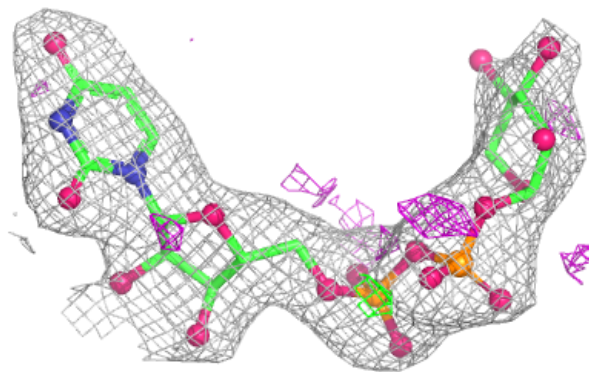
**Electron density around UDX E 500:**

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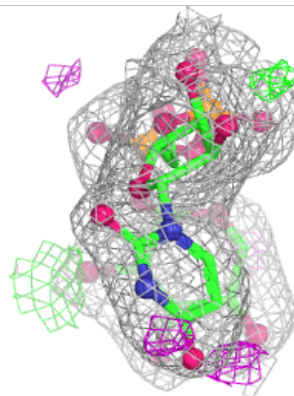
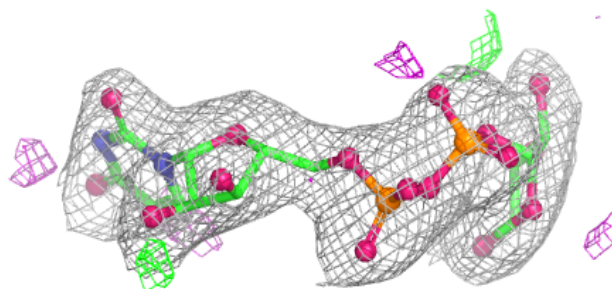
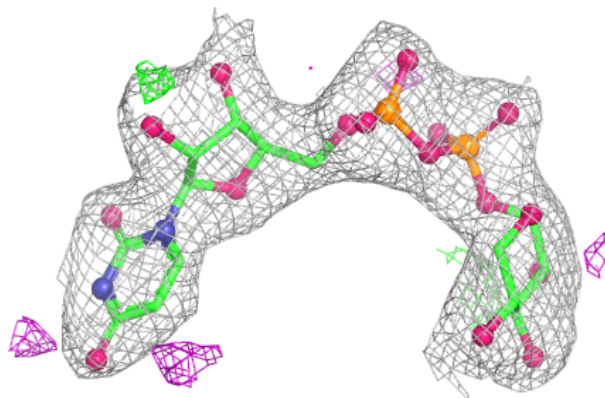


Electron density around UDX L 500:

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and green (positive)

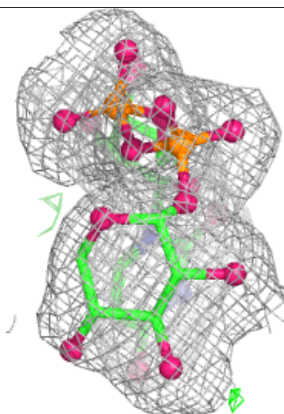
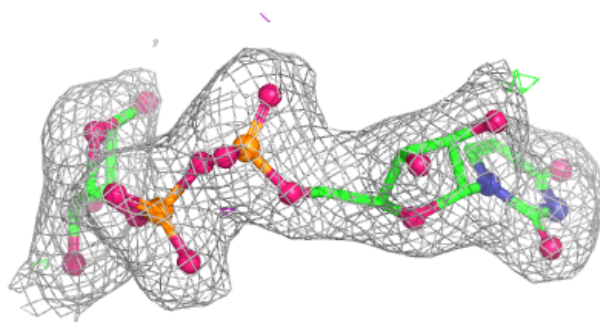
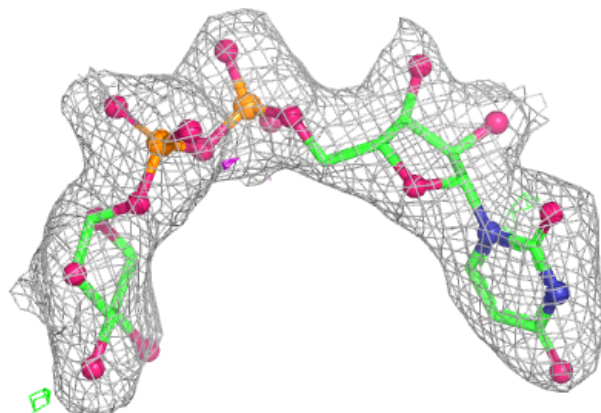
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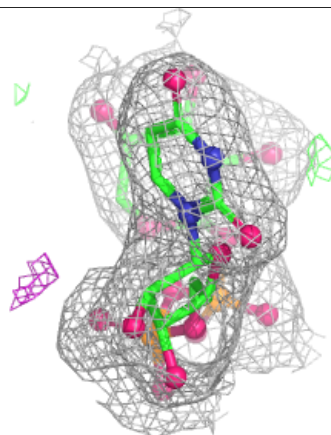
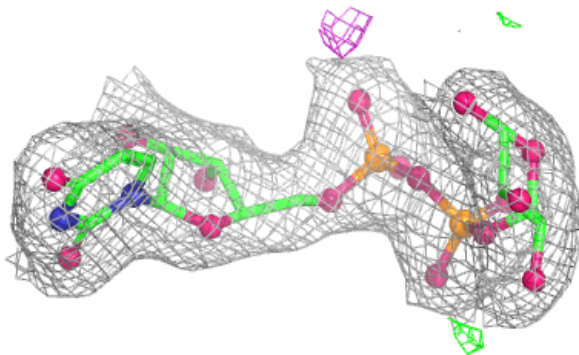
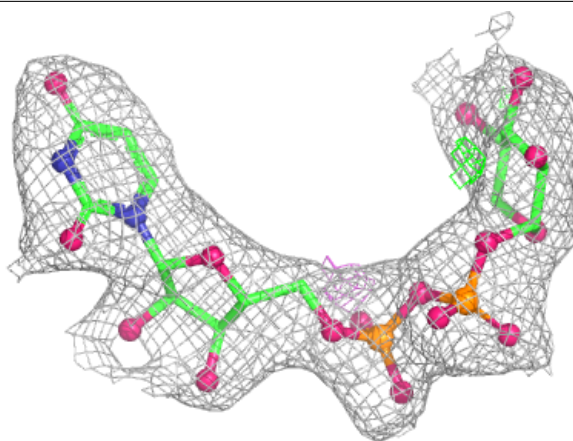
Electron density around UDX I 500:

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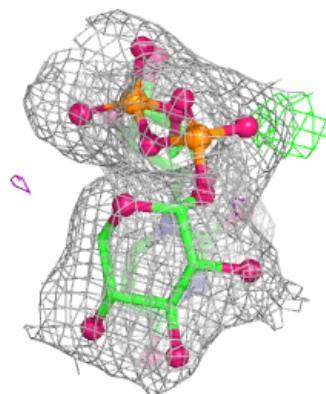
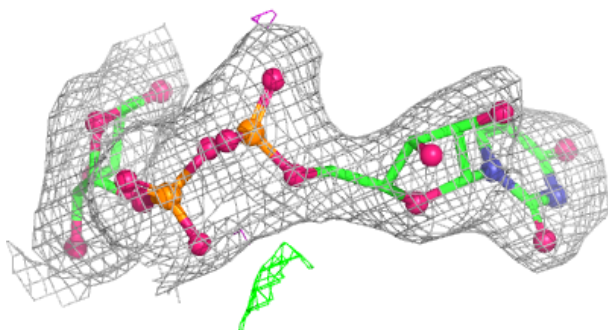
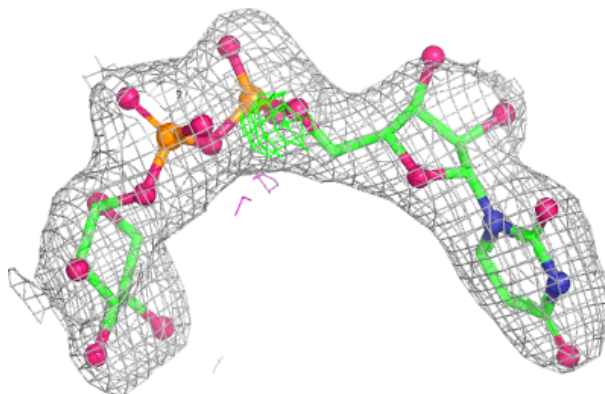


Electron density around UDX F 500:

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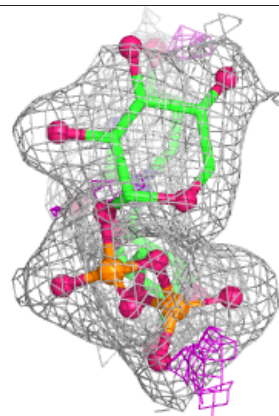
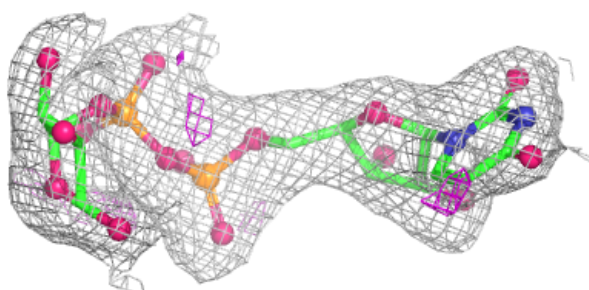
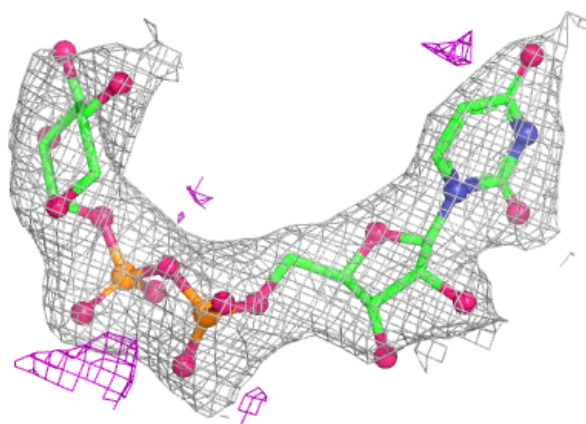
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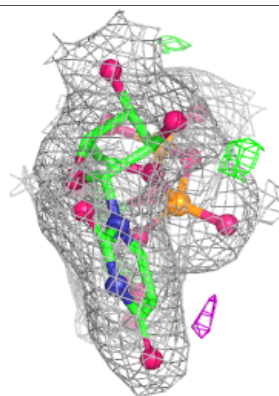
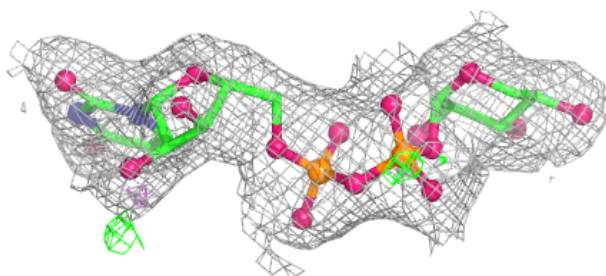
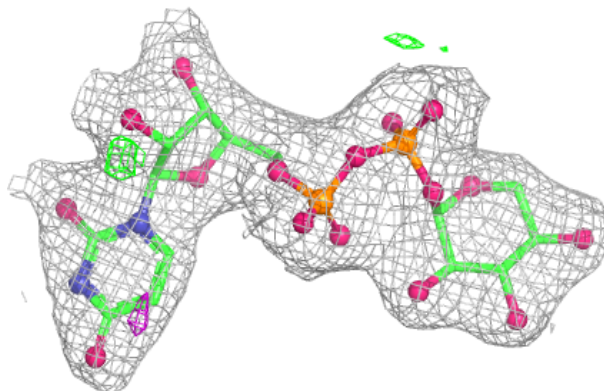


Electron density around UDX H 500:

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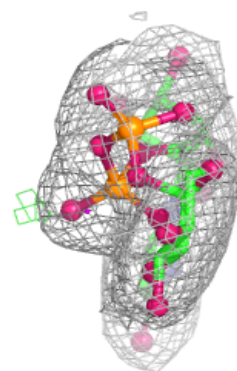
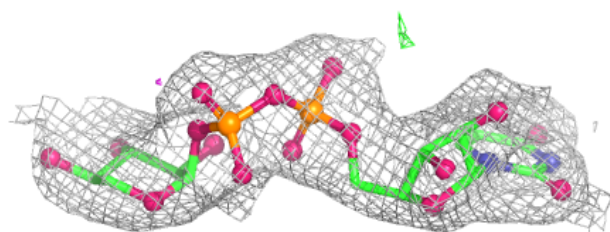
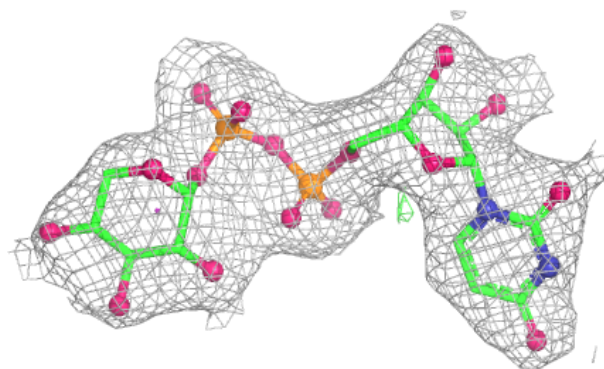
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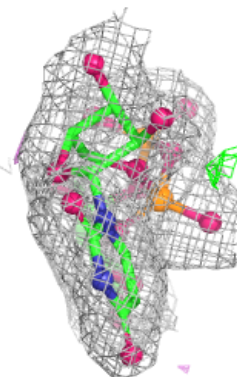
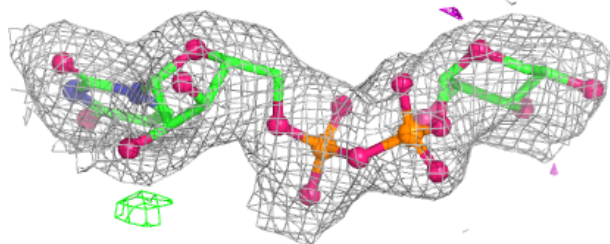
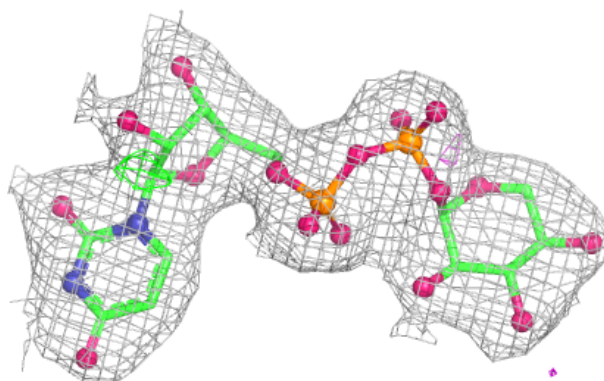


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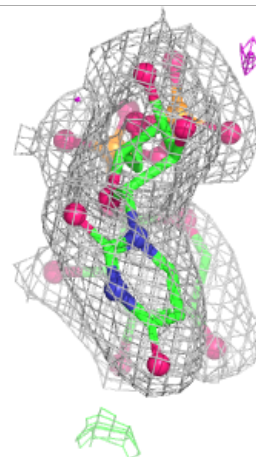
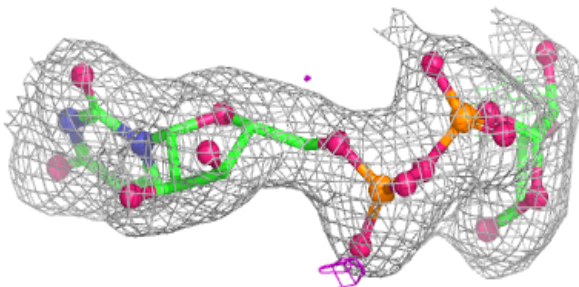
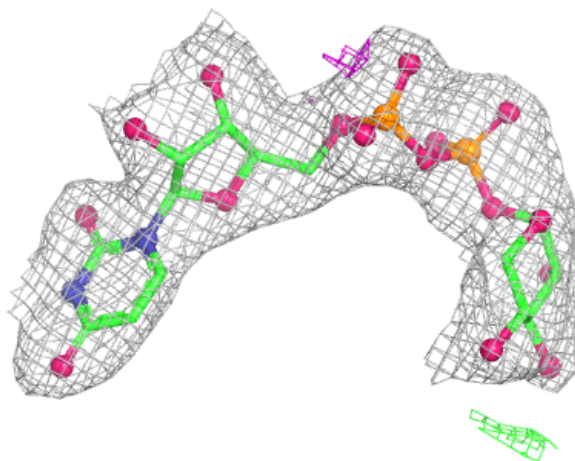
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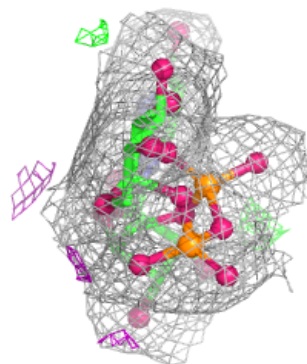
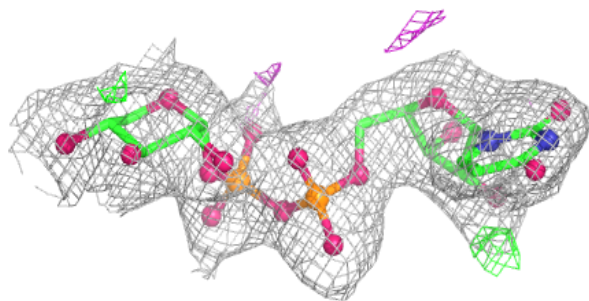
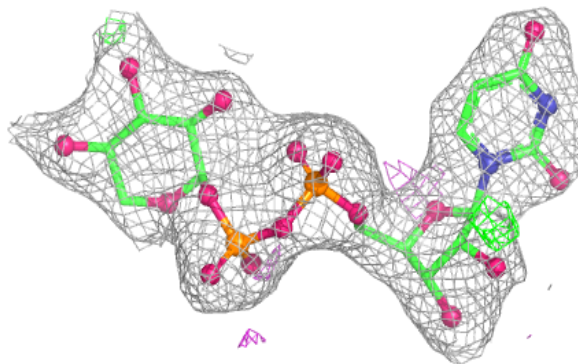
Electron density around UDX D 500:

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and green (positive)



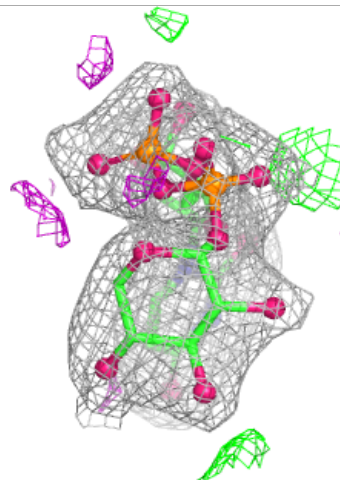
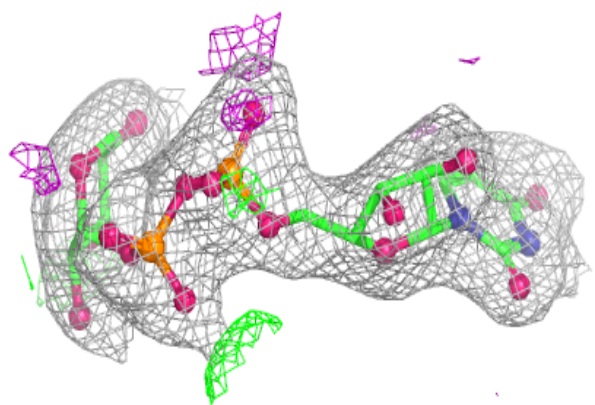
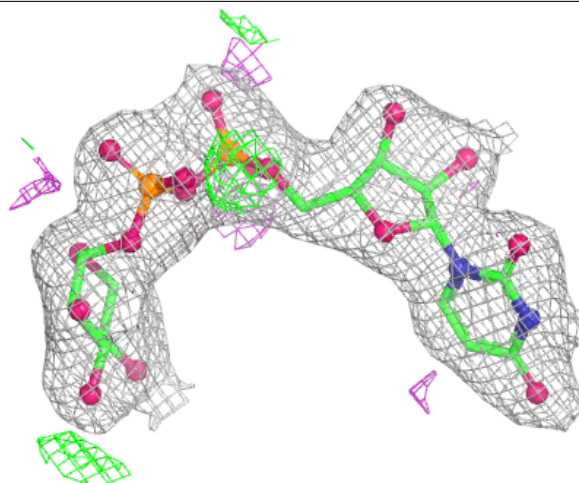
Electron density around UDX J 501:

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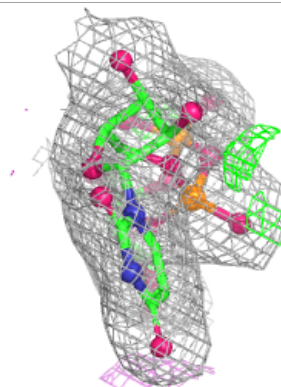
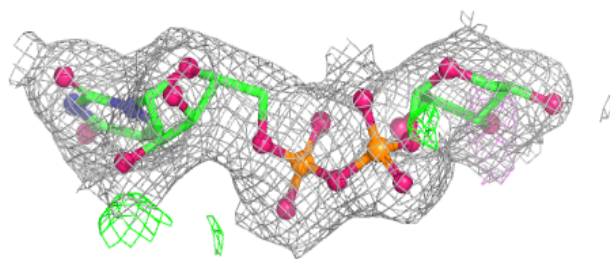
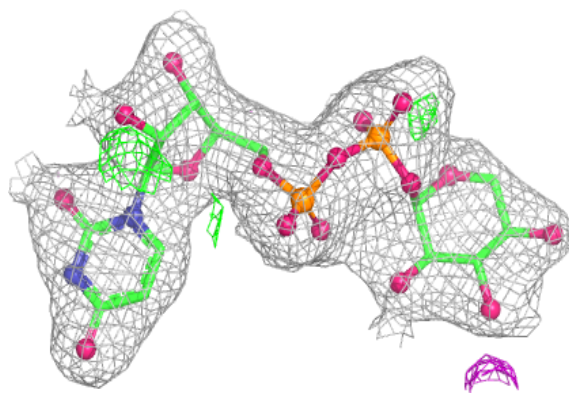
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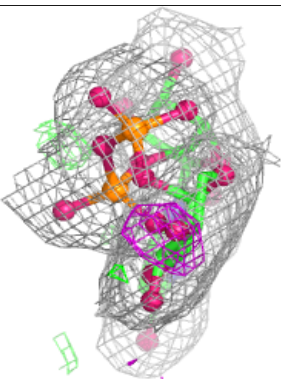
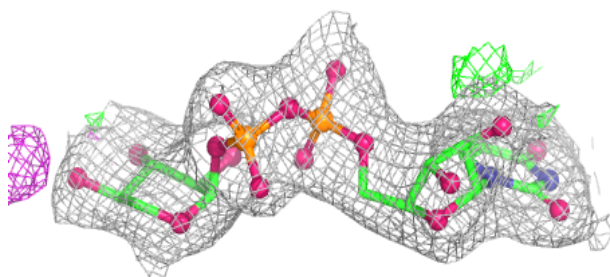
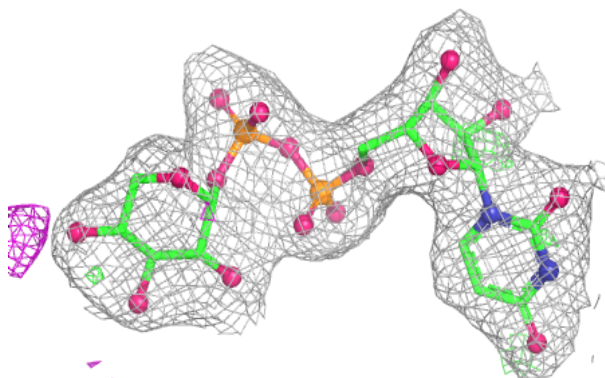


Electron density around UDX E 501:

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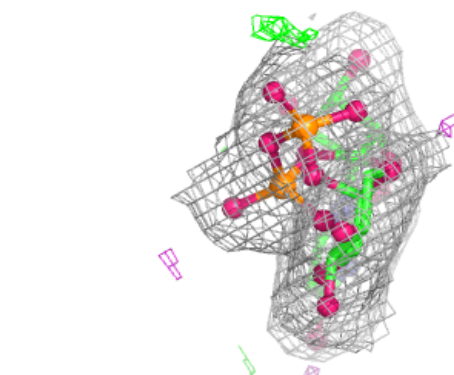
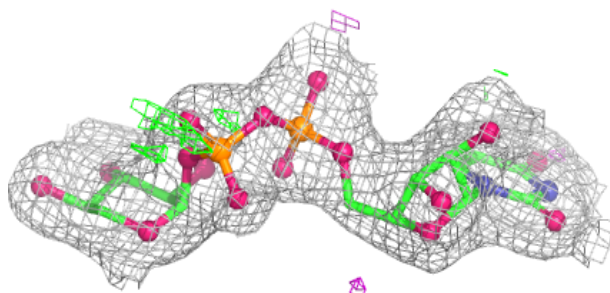
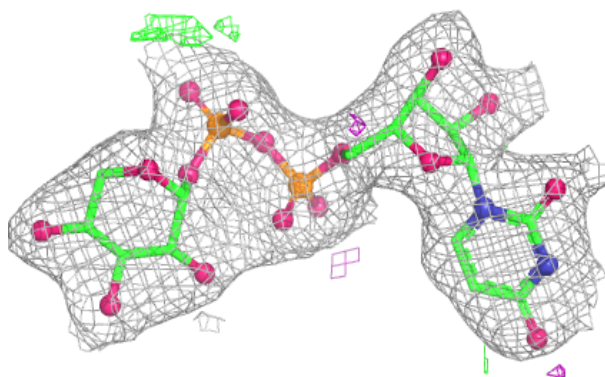
**Electron density around UDX L 501:**

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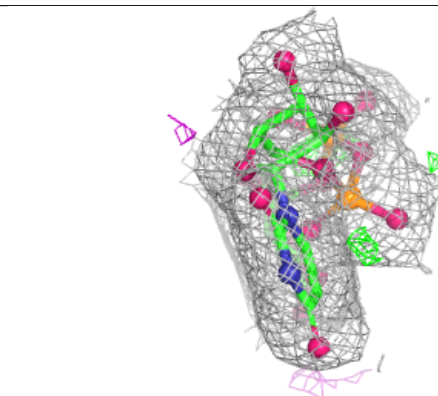
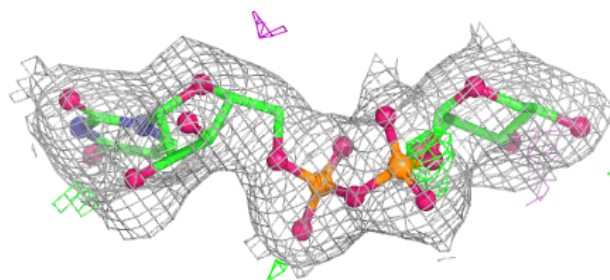
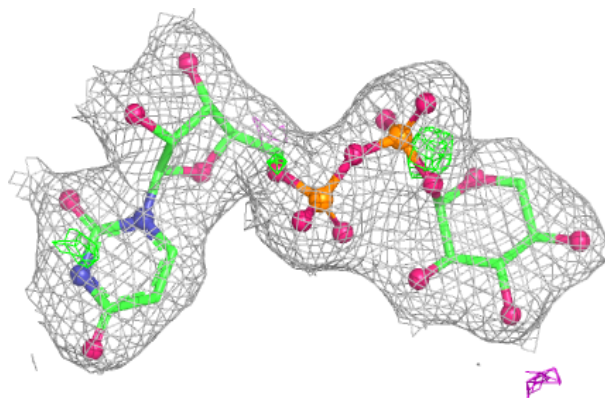


Electron density around UDX F 501:

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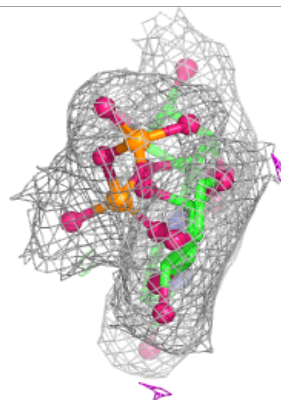
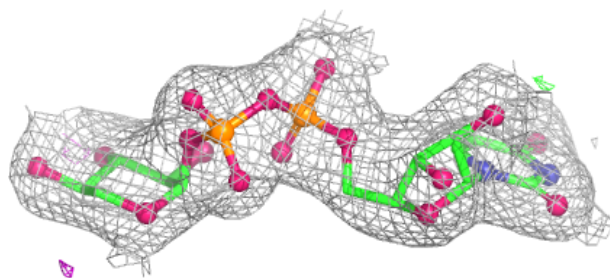
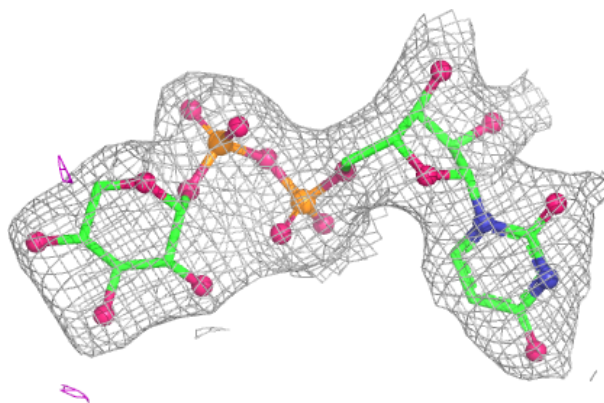
**Electron density around UDX D 501:**

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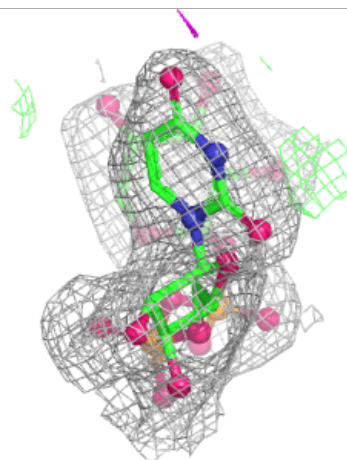
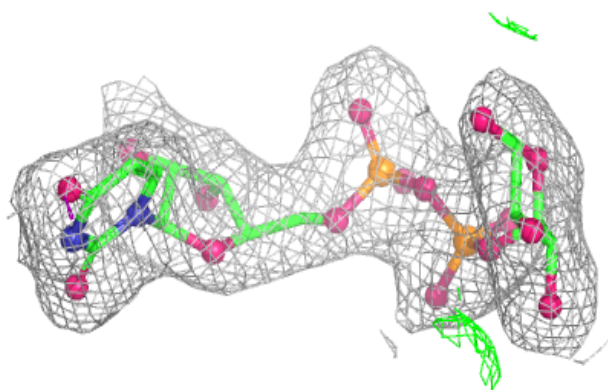
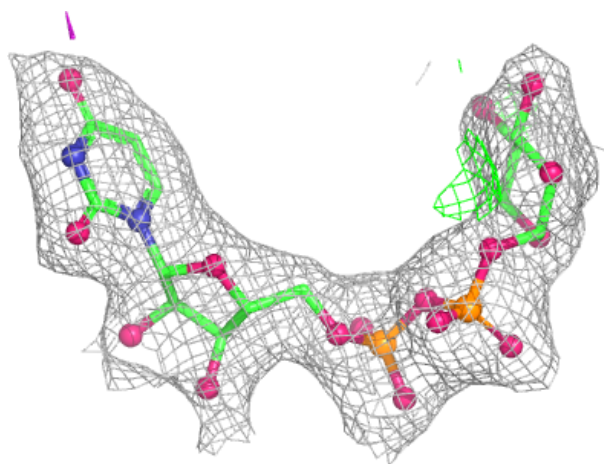
Electron density around UDX G 501:

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



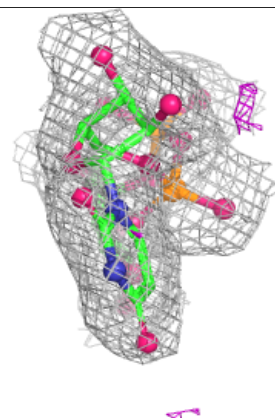
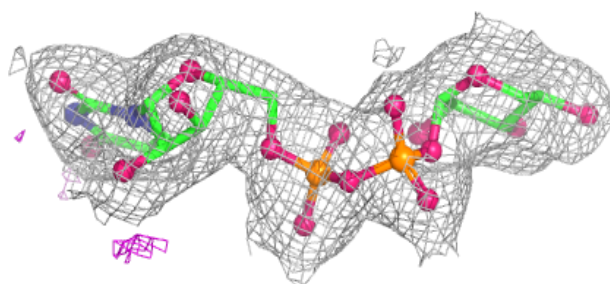
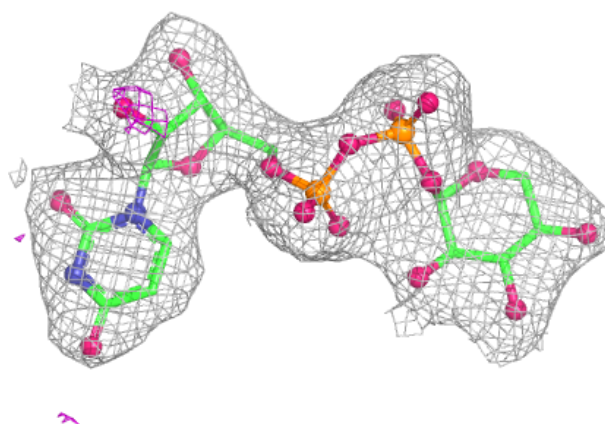
Electron density around UDX C 500:

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

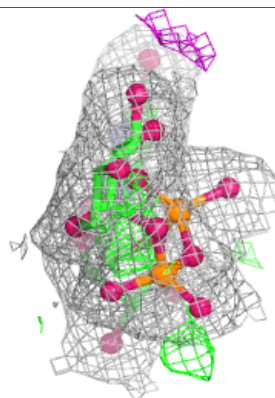
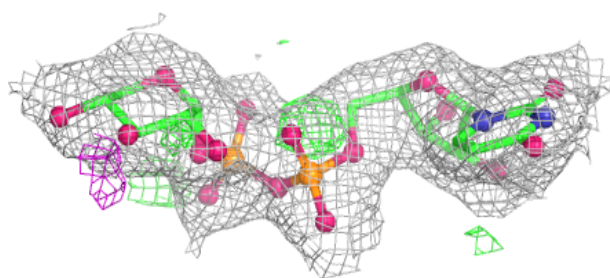
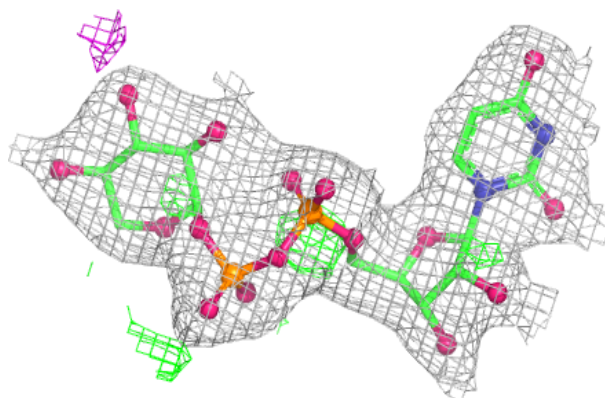


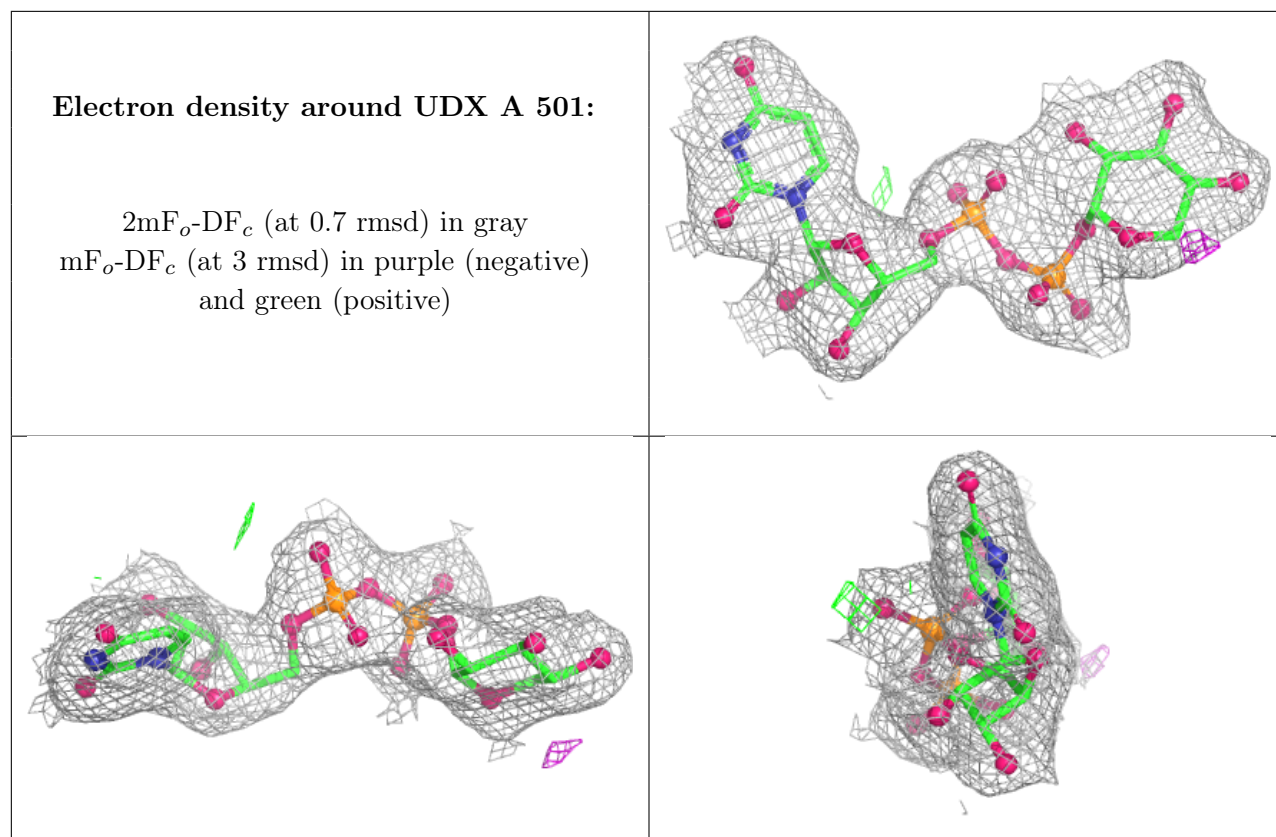
Electron density around UDX K 501:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.