



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:56 PM UTC

PDB ID : 1Q3G / pdb_00001q3g
Title : MurA (Asp305Ala) liganded with tetrahedral reaction intermediate
Authors : Eschenburg, S.; Kabsch, W.; Healy, M.L.; Schonbrunn, E.
Deposited on : 2003-07-29
Resolution : 2.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

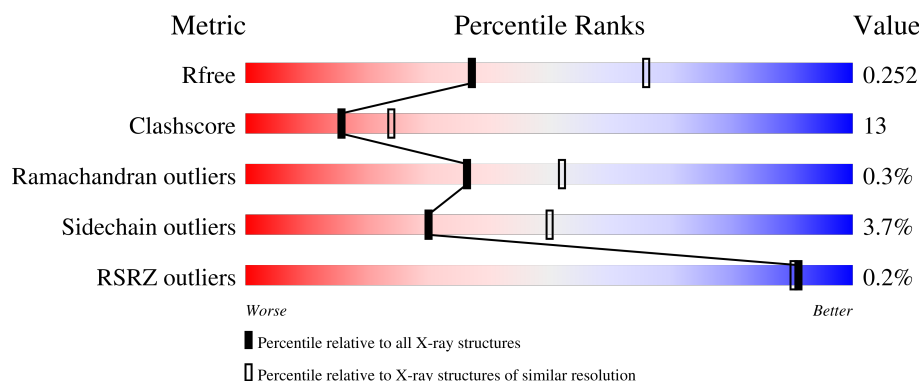
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	419	 71% 27% .
1	B	419	 72% 26% .
1	C	419	 75% 22% .
1	D	419	 72% 26% .
1	E	419	 76% 22% .

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Mol	Chain	Length	Quality of chain
1	F	419	 73%25%.
1	G	419	 74%23%.
1	H	419	 74%22%.
1	I	419	 73%25%.
1	J	419	 74%24%.
1	K	419	 74%24%.
1	L	419	 69%28%.
1	W	419	 72%26%.
1	X	419	 74%25%.
1	Y	419	 74%24%.
1	Z	419	 69%28%.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 52519 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.

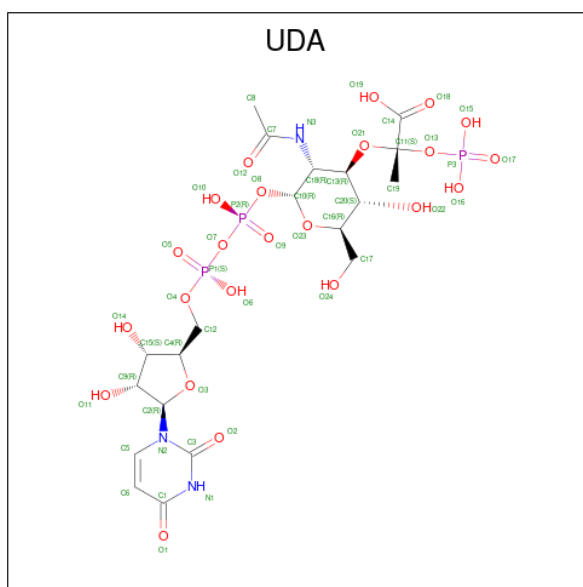
- Molecule 1 is a protein called UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	B	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	C	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	D	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	E	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	F	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	G	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	H	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	I	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	J	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	K	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	L	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	W	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	X	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	Y	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0
1	Z	419	Total 3140	C 1975	N 554	O 597	S 14	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	engineered mutation	UNP P33038
A	305	ALA	ASP	engineered mutation	UNP P33038
B	67	IAS	ASN	engineered mutation	UNP P33038
B	305	ALA	ASP	engineered mutation	UNP P33038
C	67	IAS	ASN	engineered mutation	UNP P33038
C	305	ALA	ASP	engineered mutation	UNP P33038
D	67	IAS	ASN	engineered mutation	UNP P33038
D	305	ALA	ASP	engineered mutation	UNP P33038
E	67	IAS	ASN	engineered mutation	UNP P33038
E	305	ALA	ASP	engineered mutation	UNP P33038
F	67	IAS	ASN	engineered mutation	UNP P33038
F	305	ALA	ASP	engineered mutation	UNP P33038
G	67	IAS	ASN	engineered mutation	UNP P33038
G	305	ALA	ASP	engineered mutation	UNP P33038
H	67	IAS	ASN	engineered mutation	UNP P33038
H	305	ALA	ASP	engineered mutation	UNP P33038
I	67	IAS	ASN	engineered mutation	UNP P33038
I	305	ALA	ASP	engineered mutation	UNP P33038
J	67	IAS	ASN	engineered mutation	UNP P33038
J	305	ALA	ASP	engineered mutation	UNP P33038
K	67	IAS	ASN	engineered mutation	UNP P33038
K	305	ALA	ASP	engineered mutation	UNP P33038
L	67	IAS	ASN	engineered mutation	UNP P33038
L	305	ALA	ASP	engineered mutation	UNP P33038
W	67	IAS	ASN	engineered mutation	UNP P33038
W	305	ALA	ASP	engineered mutation	UNP P33038
X	67	IAS	ASN	engineered mutation	UNP P33038
X	305	ALA	ASP	engineered mutation	UNP P33038
Y	67	IAS	ASN	engineered mutation	UNP P33038
Y	305	ALA	ASP	engineered mutation	UNP P33038
Z	67	IAS	ASN	engineered mutation	UNP P33038
Z	305	ALA	ASP	engineered mutation	UNP P33038

- Molecule 2 is 3'-1-CARBOXY-1-PHOSPHONOOXY-ETHOXY-URIDINE-DIPHOSPHAT E-N-ACETYLGLUCOSAMINE (CCD ID: UDA) (formula: $C_{20}H_{32}N_3O_{23}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	B	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	C	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	D	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	E	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	F	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	G	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	H	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	I	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	J	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	K	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	L	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	W	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	X	1	Total 49	C 20	N 3	O 23	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	Y	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	Z	1	Total	C	N	O	P	0	0
			49	20	3	23	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total C O 4 2 2	0	0
3	K	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	W	1	Total C O 4 2 2	0	0
3	X	1	Total C O 4 2 2	0	0
3	Y	1	Total C O 4 2 2	0	0
3	Z	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	93	Total O 93 93	0	0
4	B	100	Total O 100 100	0	0
4	C	124	Total O 124 124	0	0
4	D	123	Total O 123 123	0	0
4	E	116	Total O 116 116	0	0
4	F	106	Total O 106 106	0	0
4	G	136	Total O 136 136	0	0
4	H	111	Total O 111 111	0	0
4	I	76	Total O 76 76	0	0
4	J	76	Total O 76 76	0	0
4	K	67	Total O 67 67	0	0
4	L	68	Total O 68 68	0	0

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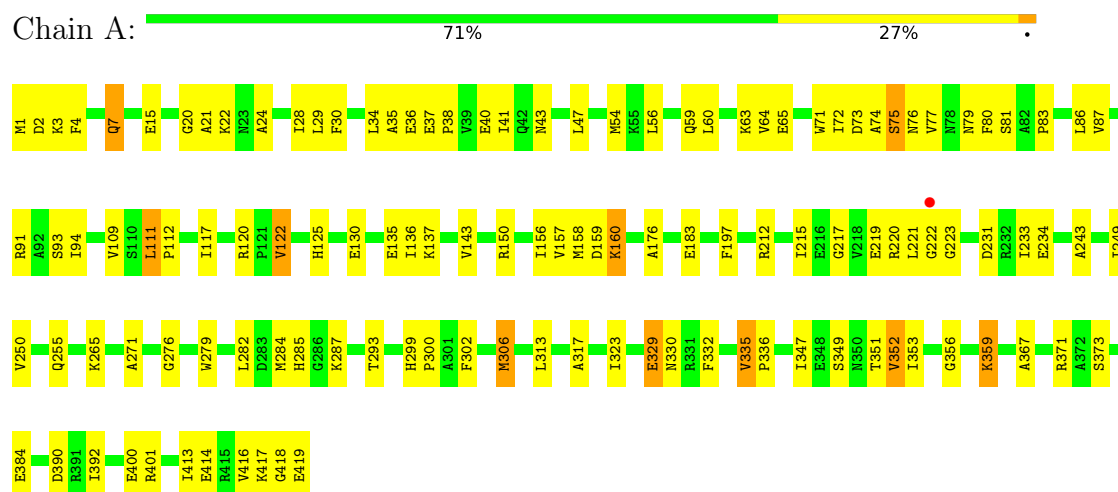
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	W	70	Total 70	O 70	0	0
4	X	52	Total 52	O 52	0	0
4	Y	67	Total 67	O 67	0	0
4	Z	46	Total 46	O 46	0	0

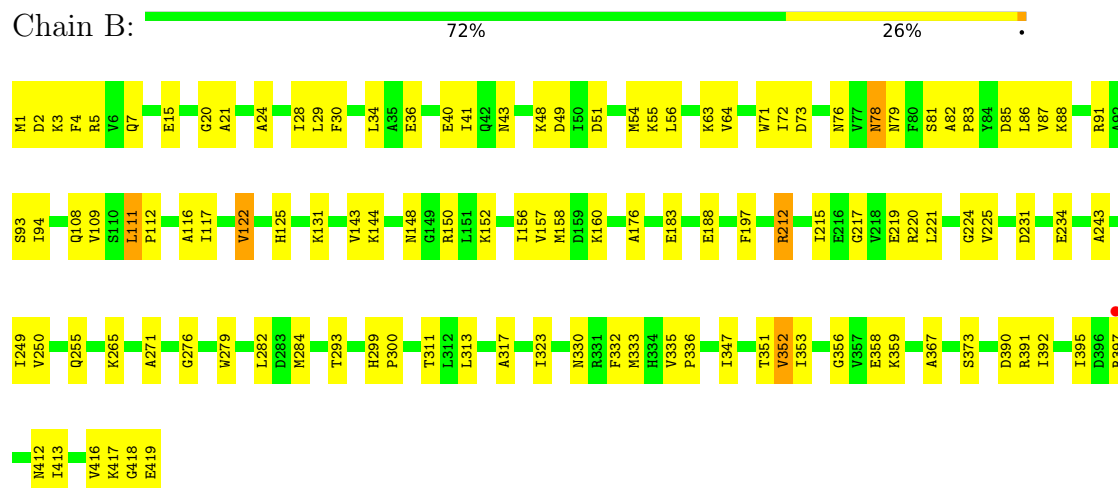
3 Residue-property plots

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-N-acetylglucosamine 1-carboxyvinyltransferase

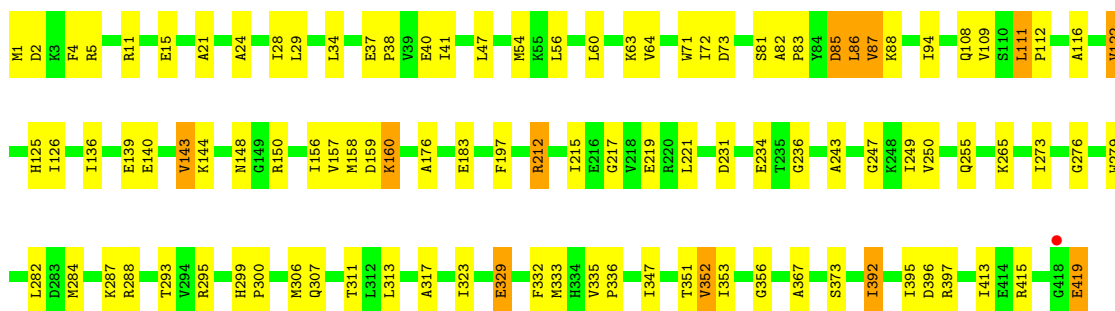


• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



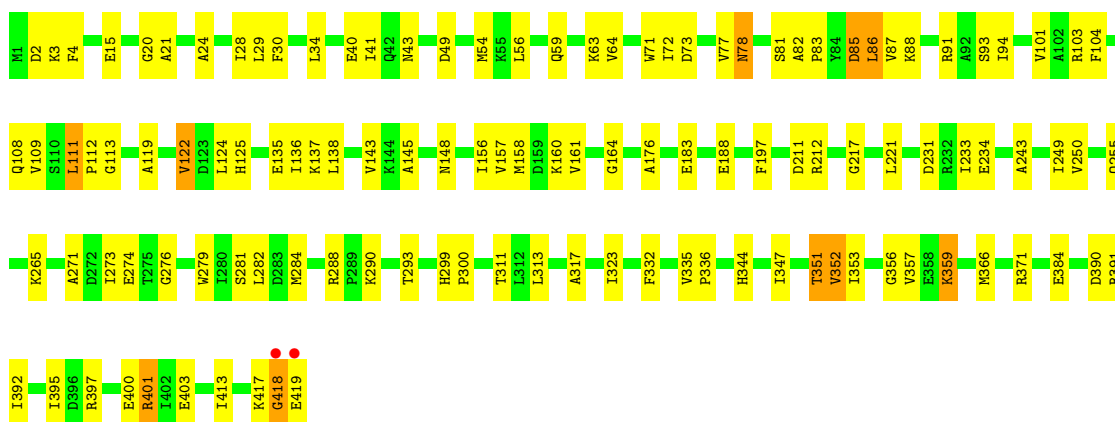
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase





- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain D: 72% 26%



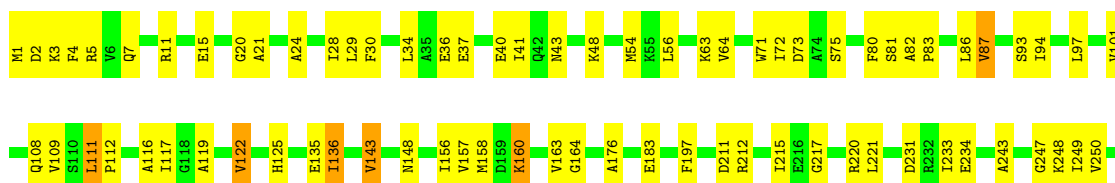
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

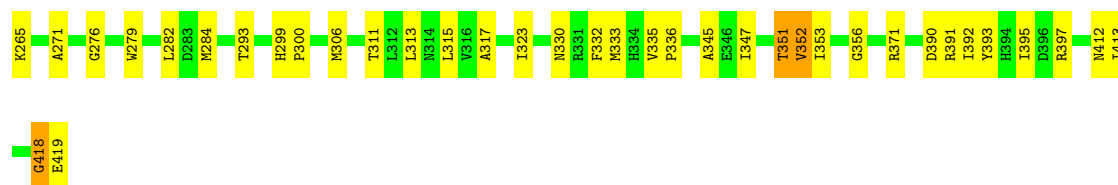
Chain E: 76% 22%



- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain F: 73% 25%





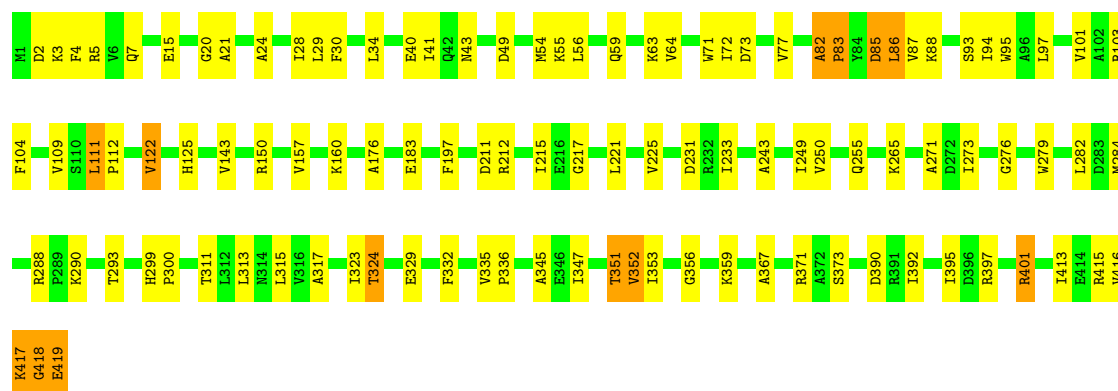
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain G: 74% 23% .



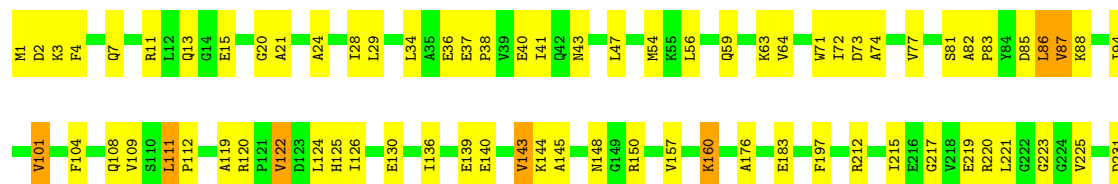
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

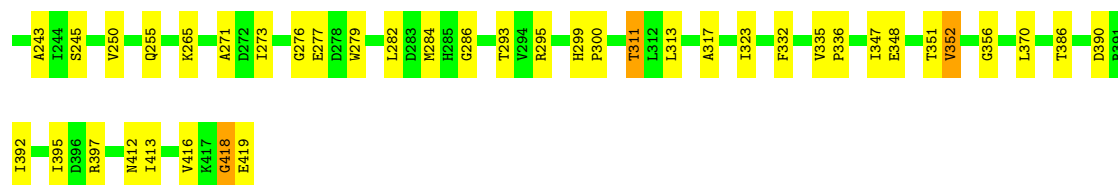
Chain H: 74% 22% .



- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

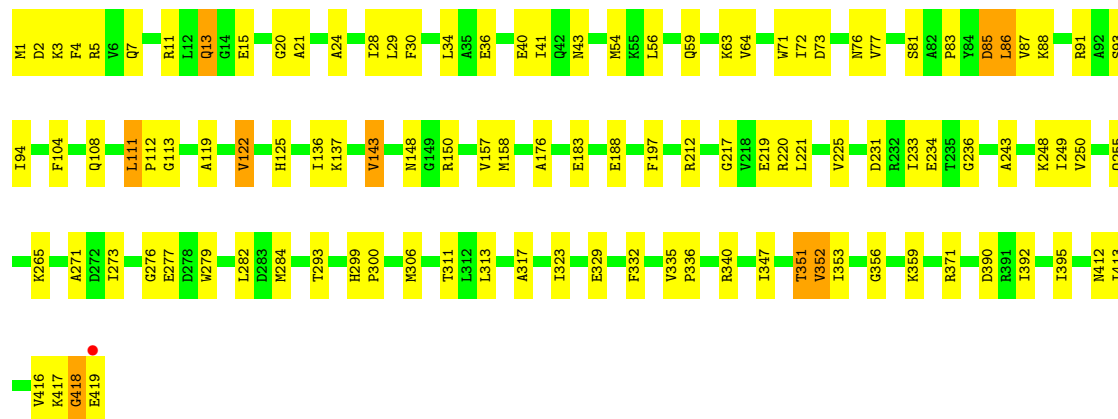
Chain I: 73% 25% .





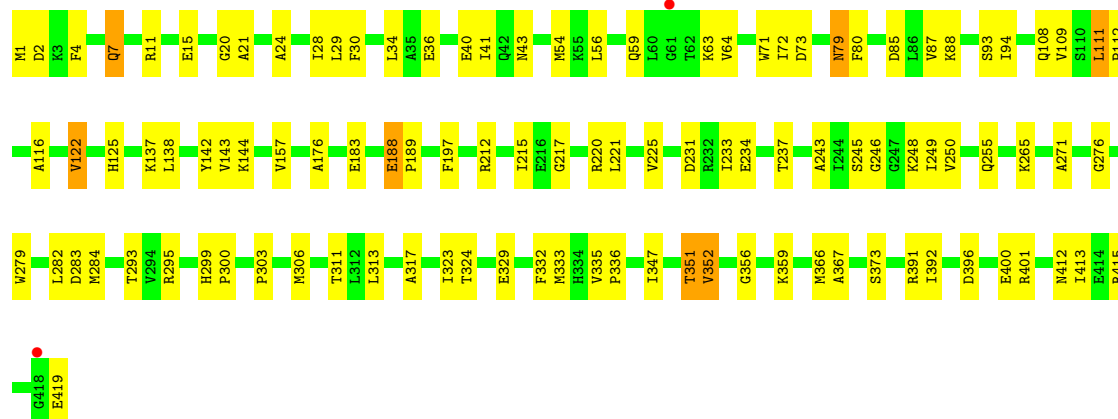
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain J: 74% 24% .



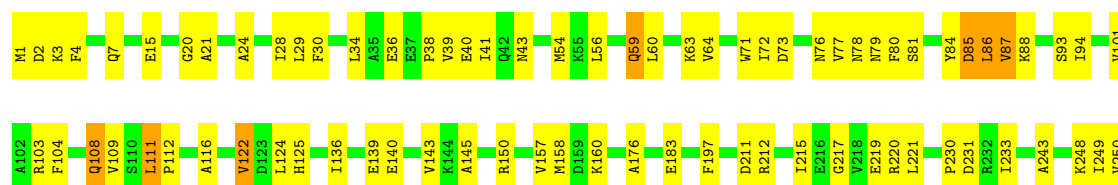
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

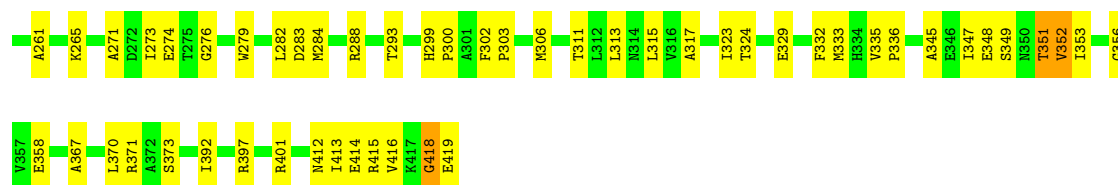
Chain K: 74% 24% .



- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

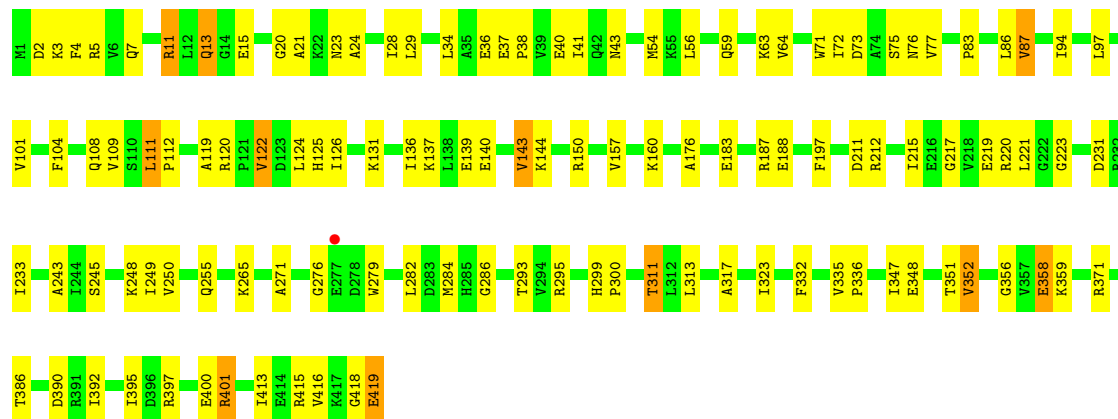
Chain L: 69% 28% .





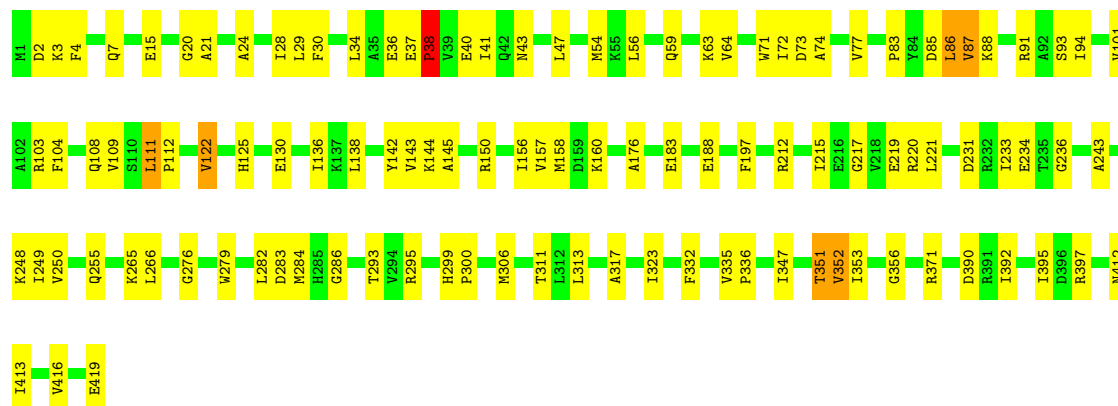
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain W: 72% 26% .



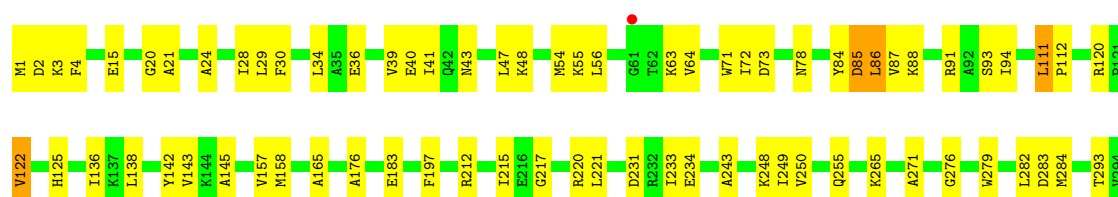
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

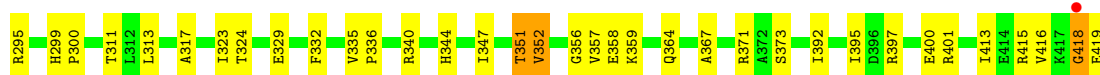
Chain X: 74% 25% .



- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

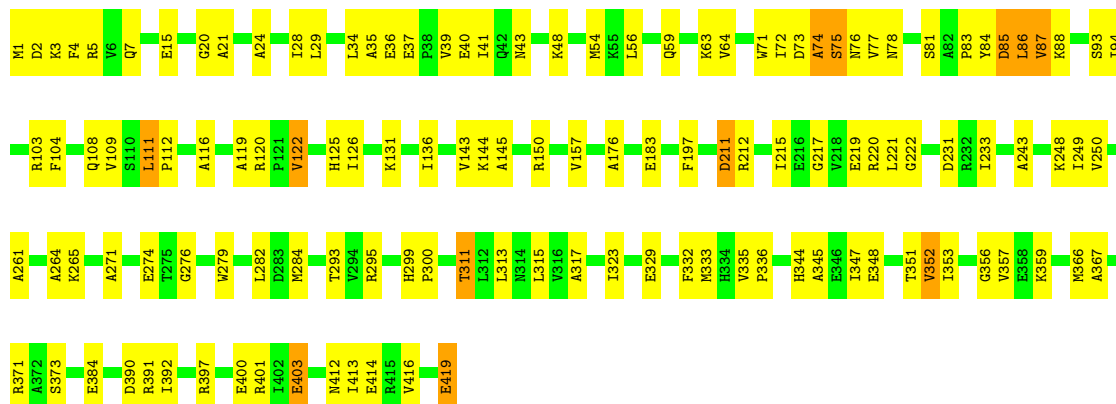
Chain Y: 74% 24% .





- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain Z: 69% 28% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	139.46Å 153.93Å 167.48Å 90.00° 112.95° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 20.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.65) 98.5 (20.00-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.253 0.216 , 0.252	Depositor DCC
R_{free} test set	3721 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52519	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3816e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: UDA, EDO, IAS

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	0.46	2/3176 (0.1%)	0.88	7/4301 (0.2%)
1	B	0.44	0/3176	0.90	6/4301 (0.1%)
1	C	0.48	0/3176	0.90	11/4301 (0.3%)
1	D	0.45	0/3176	0.91	9/4301 (0.2%)
1	E	0.46	0/3176	0.89	7/4301 (0.2%)
1	F	0.45	0/3176	0.89	4/4301 (0.1%)
1	G	0.49	1/3176 (0.0%)	0.90	10/4301 (0.2%)
1	H	0.46	0/3176	0.91	9/4301 (0.2%)
1	I	0.44	0/3176	0.90	5/4301 (0.1%)
1	J	0.43	0/3176	0.89	6/4301 (0.1%)
1	K	0.45	0/3176	0.89	8/4301 (0.2%)
1	L	0.43	0/3176	0.89	8/4301 (0.2%)
1	W	0.45	0/3176	0.89	4/4301 (0.1%)
1	X	0.43	0/3176	0.89	5/4301 (0.1%)
1	Y	0.43	0/3176	0.90	6/4301 (0.1%)
1	Z	0.43	0/3176	0.88	3/4301 (0.1%)
All	All	0.45	3/50816 (0.0%)	0.90	108/68816 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	306	MET	SD-CE	-6.13	1.64	1.79
1	A	306	MET	SD-CE	-5.30	1.66	1.79
1	A	335	VAL	CA-CB	5.05	1.56	1.54

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	ALA	N-CA-C	-7.97	103.38	113.43
1	F	24	ALA	N-CA-C	-7.96	103.39	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	82	ALA	CA-C-N	7.95	127.95	119.76
1	H	82	ALA	C-N-CA	7.95	127.95	119.76
1	E	24	ALA	N-CA-C	-7.93	103.44	113.43

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	3140	0	3217	95	0
1	B	3140	0	3217	82	0
1	C	3140	0	3217	75	0
1	D	3140	0	3217	92	0
1	E	3140	0	3217	79	0
1	F	3140	0	3217	85	0
1	G	3140	0	3217	80	0
1	H	3140	0	3217	88	0
1	I	3140	0	3217	96	0
1	J	3140	0	3217	85	0
1	K	3140	0	3217	81	0
1	L	3140	0	3217	97	0
1	W	3140	0	3217	101	0
1	X	3140	0	3217	89	0
1	Y	3140	0	3217	86	0
1	Z	3140	0	3217	105	0
2	A	49	0	28	1	0
2	B	49	0	28	0	0
2	C	49	0	28	1	0
2	D	49	0	28	0	0
2	E	49	0	28	0	0
2	F	49	0	28	0	0
2	G	49	0	28	0	0
2	H	49	0	28	0	0
2	I	49	0	28	2	0
2	J	49	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	49	0	28	0	0
2	L	49	0	28	0	0
2	W	49	0	28	1	0
2	X	49	0	28	0	0
2	Y	49	0	28	1	0
2	Z	49	0	28	1	0
3	A	4	0	6	0	0
3	B	4	0	6	1	0
3	C	4	0	6	0	0
3	D	4	0	6	3	0
3	E	4	0	6	0	0
3	F	4	0	6	2	0
3	G	4	0	6	0	0
3	H	4	0	6	0	0
3	I	4	0	6	0	0
3	J	4	0	6	0	0
3	K	4	0	6	0	0
3	L	4	0	6	0	0
3	W	4	0	6	0	0
3	X	4	0	6	1	0
3	Y	4	0	6	0	0
3	Z	4	0	6	0	0
4	A	93	0	0	2	0
4	B	100	0	0	2	0
4	C	124	0	0	1	0
4	D	123	0	0	7	0
4	E	116	0	0	0	0
4	F	106	0	0	5	0
4	G	136	0	0	5	0
4	H	111	0	0	6	0
4	I	76	0	0	0	0
4	J	76	0	0	3	0
4	K	67	0	0	2	0
4	L	68	0	0	1	0
4	W	70	0	0	2	0
4	X	52	0	0	3	0
4	Y	67	0	0	3	0
4	Z	46	0	0	2	0
All	All	52519	0	52016	1370	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 13.

The worst 5 of 1370 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:295:ARG:HD2	1:H:160:LYS:HZ3	1.18	1.05
1:G:233:ILE:HG23	1:G:306:MET:HE3	1.42	1.00
1:W:5:ARG:HH12	1:W:7:GLN:HE21	1.13	0.95
1:E:1:MET:HB3	1:E:419:GLU:HA	1.49	0.91
1:H:401:ARG:HB3	1:H:401:ARG:NH1	1.85	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/419 (99%)	402 (97%)	11 (3%)	2 (0%)	24	39
1	B	415/419 (99%)	403 (97%)	12 (3%)	0	100	100
1	C	415/419 (99%)	404 (97%)	10 (2%)	1 (0%)	43	60
1	D	415/419 (99%)	400 (96%)	14 (3%)	1 (0%)	43	60
1	E	415/419 (99%)	404 (97%)	11 (3%)	0	100	100
1	F	415/419 (99%)	402 (97%)	12 (3%)	1 (0%)	43	60
1	G	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	H	415/419 (99%)	405 (98%)	8 (2%)	2 (0%)	24	39
1	I	415/419 (99%)	402 (97%)	11 (3%)	2 (0%)	24	39
1	J	415/419 (99%)	403 (97%)	11 (3%)	1 (0%)	43	60
1	K	415/419 (99%)	401 (97%)	14 (3%)	0	100	100
1	L	415/419 (99%)	400 (96%)	13 (3%)	2 (0%)	24	39
1	W	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	X	415/419 (99%)	403 (97%)	11 (3%)	1 (0%)	43	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Y	415/419 (99%)	402 (97%)	11 (3%)	2 (0%)	24 39
1	Z	415/419 (99%)	403 (97%)	9 (2%)	3 (1%)	18 30
All	All	6640/6704 (99%)	6438 (97%)	184 (3%)	18 (0%)	36 52

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	F	418	GLY
1	L	418	GLY
1	A	160	LYS
1	C	160	LYS

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	328/328 (100%)	318 (97%)	10 (3%)	36 57
1	B	328/328 (100%)	316 (96%)	12 (4%)	30 50
1	C	328/328 (100%)	315 (96%)	13 (4%)	28 47
1	D	328/328 (100%)	312 (95%)	16 (5%)	22 38
1	E	328/328 (100%)	316 (96%)	12 (4%)	30 50
1	F	328/328 (100%)	318 (97%)	10 (3%)	36 57
1	G	328/328 (100%)	316 (96%)	12 (4%)	30 50
1	H	328/328 (100%)	316 (96%)	12 (4%)	30 50
1	I	328/328 (100%)	316 (96%)	12 (4%)	30 50
1	J	328/328 (100%)	315 (96%)	13 (4%)	28 47
1	K	328/328 (100%)	317 (97%)	11 (3%)	32 53
1	L	328/328 (100%)	310 (94%)	18 (6%)	19 33
1	W	328/328 (100%)	314 (96%)	14 (4%)	26 44
1	X	328/328 (100%)	320 (98%)	8 (2%)	43 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	328/328 (100%)	319 (97%)	9 (3%)	39	61
1	Z	328/328 (100%)	315 (96%)	13 (4%)	28	47
All	All	5248/5248 (100%)	5053 (96%)	195 (4%)	30	50

5 of 195 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	111	LEU
1	L	158	MET
1	J	212	ARG
1	K	351	THR
1	L	414	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	148	ASN
1	Z	299	HIS
1	J	394	HIS
1	Z	285	HIS
1	Y	76	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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
1	IAS	J	67	1	6,7,8	0.93	0	3,8,10	1.05	0
1	IAS	G	67	1	6,7,8	0.97	0	3,8,10	1.17	0
1	IAS	Y	67	1	6,7,8	0.98	0	3,8,10	1.07	0
1	IAS	D	67	1	6,7,8	0.90	0	3,8,10	1.07	0
1	IAS	H	67	1	6,7,8	0.96	0	3,8,10	0.96	0
1	IAS	B	67	1	6,7,8	0.97	0	3,8,10	0.99	0
1	IAS	K	67	1	6,7,8	0.97	0	3,8,10	1.01	0
1	IAS	L	67	1	6,7,8	0.92	0	3,8,10	1.14	0
1	IAS	F	67	1	6,7,8	0.92	0	3,8,10	1.00	0
1	IAS	X	67	1	6,7,8	0.95	0	3,8,10	1.03	0
1	IAS	E	67	1	6,7,8	0.93	0	3,8,10	1.06	0
1	IAS	Z	67	1	6,7,8	0.91	0	3,8,10	1.07	0
1	IAS	I	67	1	6,7,8	0.99	0	3,8,10	0.96	0
1	IAS	W	67	1	6,7,8	1.04	0	3,8,10	0.94	0
1	IAS	C	67	1	6,7,8	0.92	0	3,8,10	1.11	0
1	IAS	A	67	1	6,7,8	0.95	0	3,8,10	1.09	0

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
1	IAS	J	67	1	-	0/7/7/8	-
1	IAS	G	67	1	-	0/7/7/8	-
1	IAS	Y	67	1	-	0/7/7/8	-
1	IAS	D	67	1	-	0/7/7/8	-
1	IAS	H	67	1	-	0/7/7/8	-
1	IAS	B	67	1	-	0/7/7/8	-
1	IAS	K	67	1	-	0/7/7/8	-
1	IAS	L	67	1	-	0/7/7/8	-
1	IAS	F	67	1	-	0/7/7/8	-
1	IAS	X	67	1	-	0/7/7/8	-
1	IAS	E	67	1	-	0/7/7/8	-
1	IAS	Z	67	1	-	0/7/7/8	-
1	IAS	I	67	1	-	0/7/7/8	-
1	IAS	W	67	1	-	0/7/7/8	-
1	IAS	C	67	1	-	0/7/7/8	-
1	IAS	A	67	1	-	0/7/7/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

32 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	UDA	C	1452	-	48,51,51	2.59	19 (39%)	68,79,79	1.67	17 (25%)
3	EDO	F	1475	-	3,3,3	0.78	0	2,2,2	0.22	0
2	UDA	J	1459	-	48,51,51	2.41	21 (43%)	68,79,79	1.66	13 (19%)
3	EDO	D	1473	-	3,3,3	0.80	0	2,2,2	0.52	0
3	EDO	Y	1484	-	3,3,3	0.42	0	2,2,2	0.11	0
3	EDO	G	1476	-	3,3,3	0.54	0	2,2,2	0.19	0
3	EDO	A	1470	-	3,3,3	0.54	0	2,2,2	0.20	0
2	UDA	H	1457	-	48,51,51	2.53	20 (41%)	68,79,79	1.68	15 (22%)
3	EDO	C	1472	-	3,3,3	0.48	0	2,2,2	0.11	0
2	UDA	B	1451	-	48,51,51	2.45	22 (45%)	68,79,79	1.68	18 (26%)
2	UDA	D	1453	-	48,51,51	2.59	20 (41%)	68,79,79	1.64	14 (20%)
2	UDA	K	1460	-	48,51,51	2.50	21 (43%)	68,79,79	1.69	18 (26%)
2	UDA	G	1456	-	48,51,51	2.38	19 (39%)	68,79,79	1.69	19 (27%)
2	UDA	Z	1465	-	48,51,51	2.44	22 (45%)	68,79,79	1.64	16 (23%)
3	EDO	W	1482	-	3,3,3	0.48	0	2,2,2	0.20	0
3	EDO	I	1478	-	3,3,3	0.54	0	2,2,2	0.21	0
2	UDA	L	1461	-	48,51,51	2.34	21 (43%)	68,79,79	1.69	16 (23%)
3	EDO	H	1477	-	3,3,3	0.39	0	2,2,2	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	J	1479	-	3,3,3	0.57	0	2,2,2	0.24	0
2	UDA	I	1458	-	48,51,51	2.45	20 (41%)	68,79,79	1.59	14 (20%)
2	UDA	Y	1464	-	48,51,51	2.56	19 (39%)	68,79,79	1.62	15 (22%)
3	EDO	K	1480	-	3,3,3	0.39	0	2,2,2	0.02	0
3	EDO	L	1481	-	3,3,3	0.54	0	2,2,2	0.14	0
3	EDO	B	1471	-	3,3,3	0.46	0	2,2,2	0.09	0
2	UDA	W	1462	-	48,51,51	2.33	19 (39%)	68,79,79	1.61	14 (20%)
3	EDO	Z	1485	-	3,3,3	0.57	0	2,2,2	0.21	0
2	UDA	E	1454	-	48,51,51	2.50	19 (39%)	68,79,79	1.67	17 (25%)
2	UDA	F	1455	-	48,51,51	2.47	22 (45%)	68,79,79	1.70	17 (25%)
3	EDO	X	1483	-	3,3,3	0.45	0	2,2,2	0.13	0
3	EDO	E	1474	-	3,3,3	0.36	0	2,2,2	0.11	0
2	UDA	X	1463	-	48,51,51	2.33	20 (41%)	68,79,79	1.68	18 (26%)
2	UDA	A	1450	-	48,51,51	2.45	21 (43%)	68,79,79	1.70	16 (23%)

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	UDA	C	1452	-	-	9/35/80/80	0/3/3/3
3	EDO	F	1475	-	-	1/1/1/1	-
2	UDA	J	1459	-	-	7/35/80/80	0/3/3/3
3	EDO	D	1473	-	-	1/1/1/1	-
3	EDO	Y	1484	-	-	1/1/1/1	-
3	EDO	G	1476	-	-	1/1/1/1	-
3	EDO	A	1470	-	-	1/1/1/1	-
2	UDA	H	1457	-	-	8/35/80/80	0/3/3/3
3	EDO	C	1472	-	-	1/1/1/1	-
2	UDA	B	1451	-	-	8/35/80/80	0/3/3/3
2	UDA	D	1453	-	-	8/35/80/80	0/3/3/3
2	UDA	K	1460	-	-	9/35/80/80	0/3/3/3
2	UDA	G	1456	-	-	9/35/80/80	0/3/3/3
2	UDA	Z	1465	-	-	8/35/80/80	0/3/3/3
3	EDO	W	1482	-	-	1/1/1/1	-
3	EDO	I	1478	-	-	1/1/1/1	-
2	UDA	L	1461	-	-	8/35/80/80	0/3/3/3
3	EDO	H	1477	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	J	1479	-	-	1/1/1/1	-
2	UDA	I	1458	-	-	8/35/80/80	0/3/3/3
2	UDA	Y	1464	-	-	8/35/80/80	0/3/3/3
3	EDO	K	1480	-	-	1/1/1/1	-
3	EDO	L	1481	-	-	1/1/1/1	-
3	EDO	B	1471	-	-	1/1/1/1	-
2	UDA	W	1462	-	-	8/35/80/80	0/3/3/3
3	EDO	Z	1485	-	-	1/1/1/1	-
2	UDA	E	1454	-	-	7/35/80/80	0/3/3/3
2	UDA	F	1455	-	-	9/35/80/80	0/3/3/3
3	EDO	X	1483	-	-	1/1/1/1	-
3	EDO	E	1474	-	-	1/1/1/1	-
2	UDA	X	1463	-	-	7/35/80/80	0/3/3/3
2	UDA	A	1450	-	-	9/35/80/80	0/3/3/3

The worst 5 of 325 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1453	UDA	P1-O7	-10.04	1.48	1.59
2	C	1452	UDA	P1-O7	-9.81	1.48	1.59
2	I	1458	UDA	P1-O7	-9.43	1.49	1.59
2	K	1460	UDA	P1-O7	-9.06	1.49	1.59
2	Y	1464	UDA	P1-O7	-9.02	1.49	1.59

The worst 5 of 257 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1458	UDA	O14-C15-C4	4.05	122.72	111.08
2	H	1457	UDA	O14-C15-C4	4.02	122.64	111.08
2	H	1457	UDA	O7-P1-O5	-3.99	98.70	110.70
2	D	1453	UDA	O14-C15-C4	3.99	122.53	111.08
2	D	1453	UDA	O7-P1-O5	-3.90	98.98	110.70

There are no chirality outliers.

5 of 146 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1450	UDA	C12-O4-P1-O5
2	A	1450	UDA	C12-O4-P1-O6
2	A	1450	UDA	C12-O4-P1-O7

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Mol	Chain	Res	Type	Atoms
2	A	1450	UDA	O21-C11-C14-O18
2	A	1450	UDA	O21-C11-C14-O19

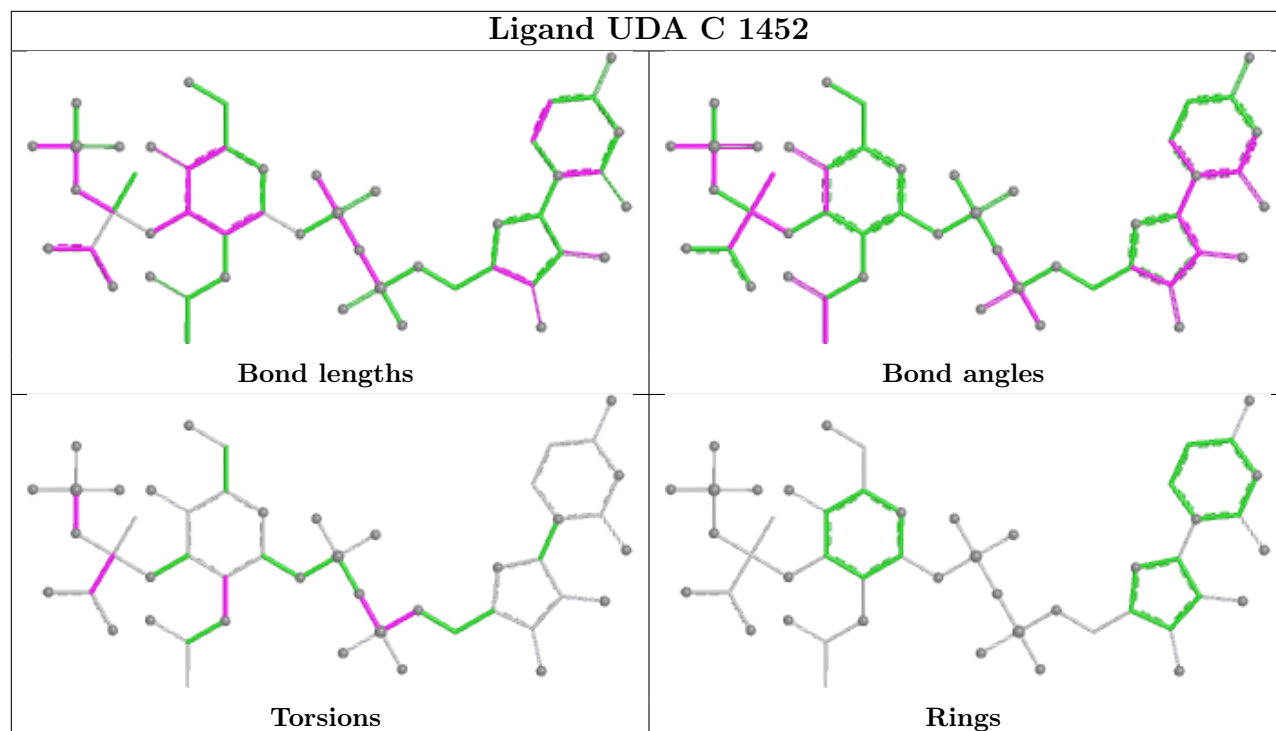
There are no ring outliers.

10 monomers are involved in 14 short contacts:

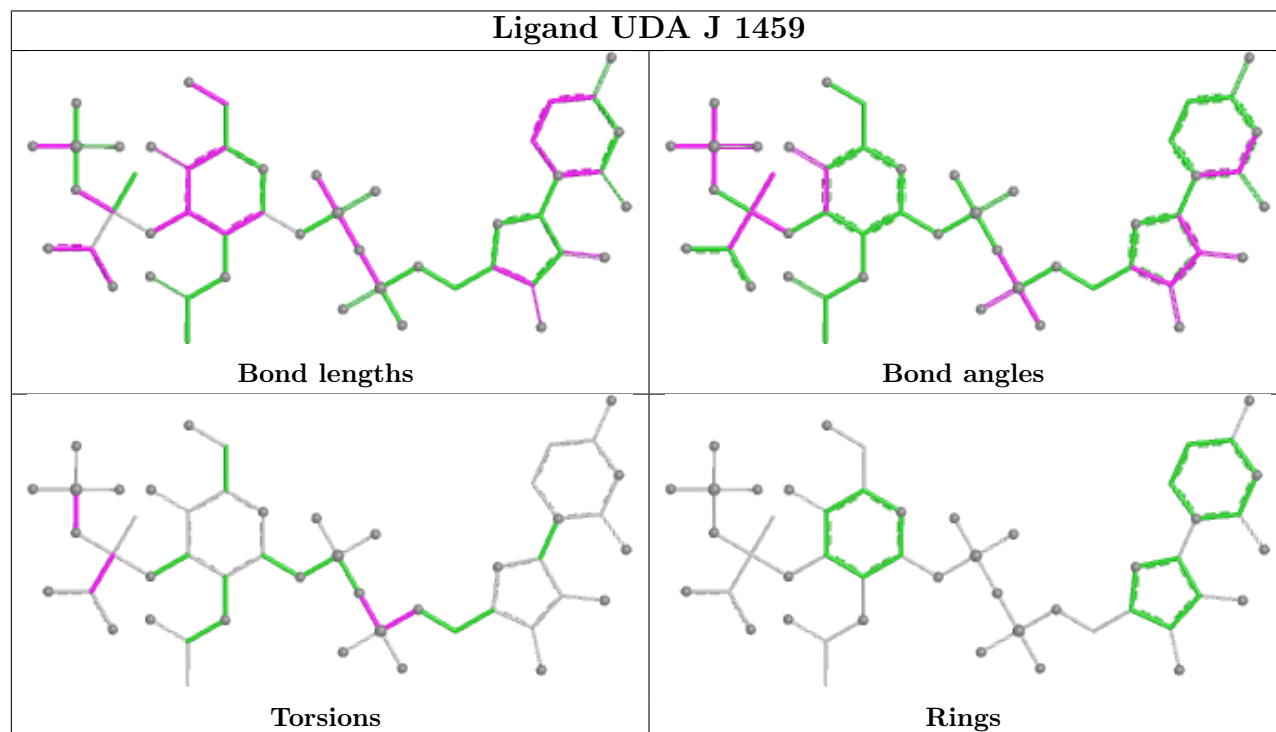
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1452	UDA	1	0
3	F	1475	EDO	2	0
3	D	1473	EDO	3	0
2	Z	1465	UDA	1	0
2	I	1458	UDA	2	0
2	Y	1464	UDA	1	0
3	B	1471	EDO	1	0
2	W	1462	UDA	1	0
3	X	1483	EDO	1	0
2	A	1450	UDA	1	0

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.

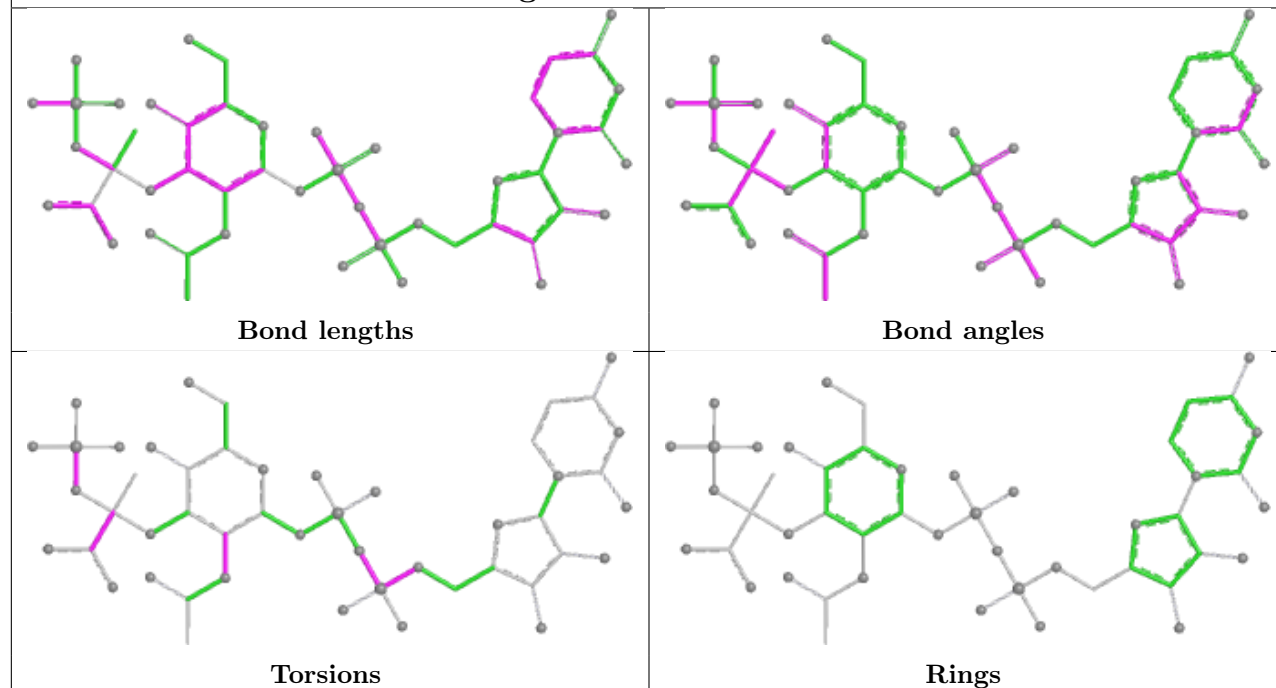
Ligand UDA C 1452



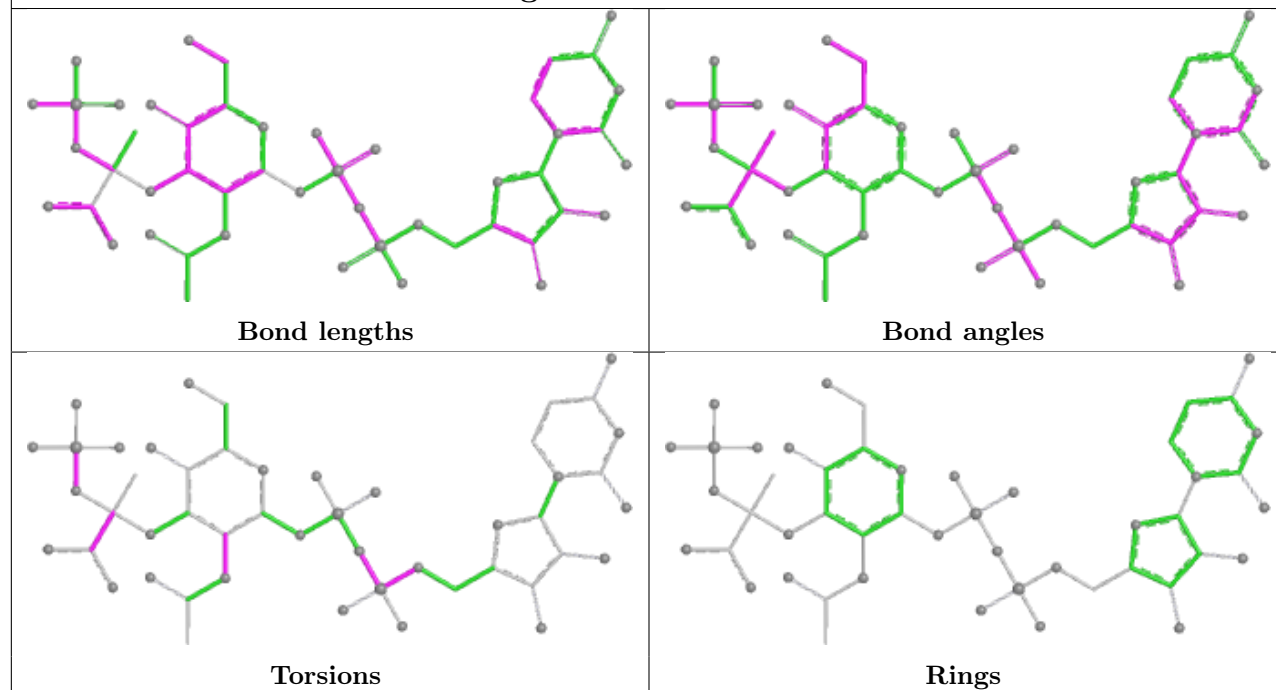
Ligand UDA J 1459



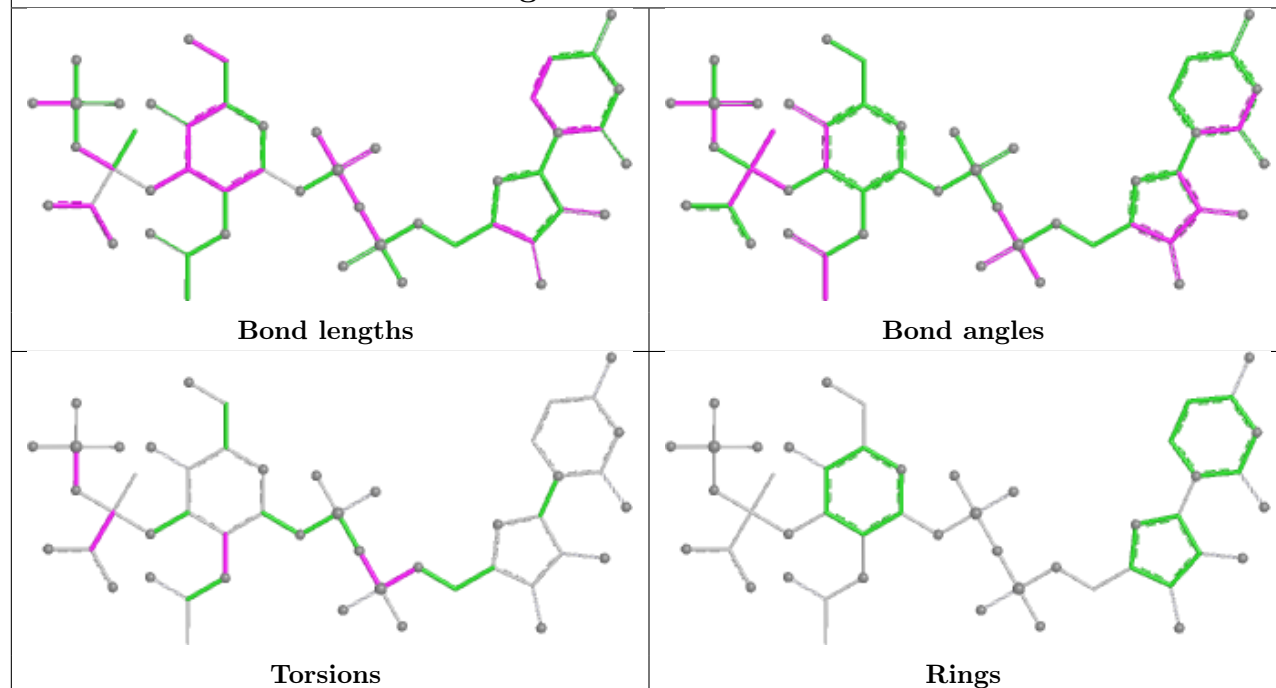
Ligand UDA H 1457



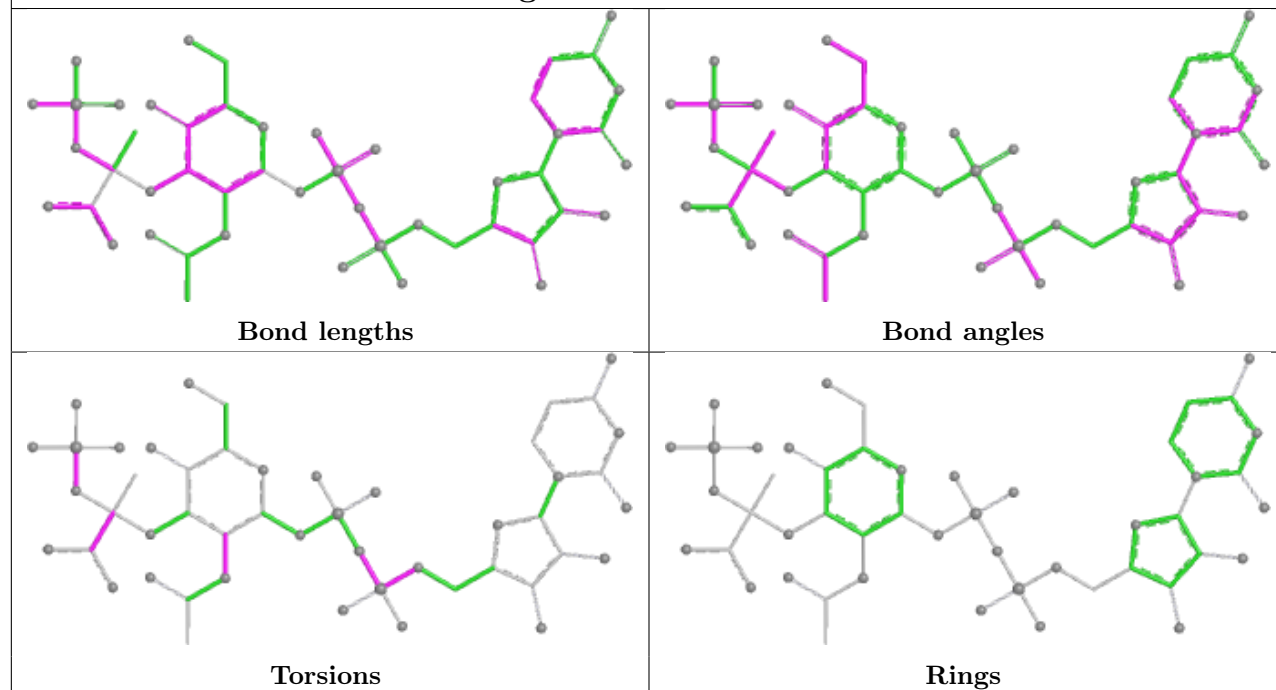
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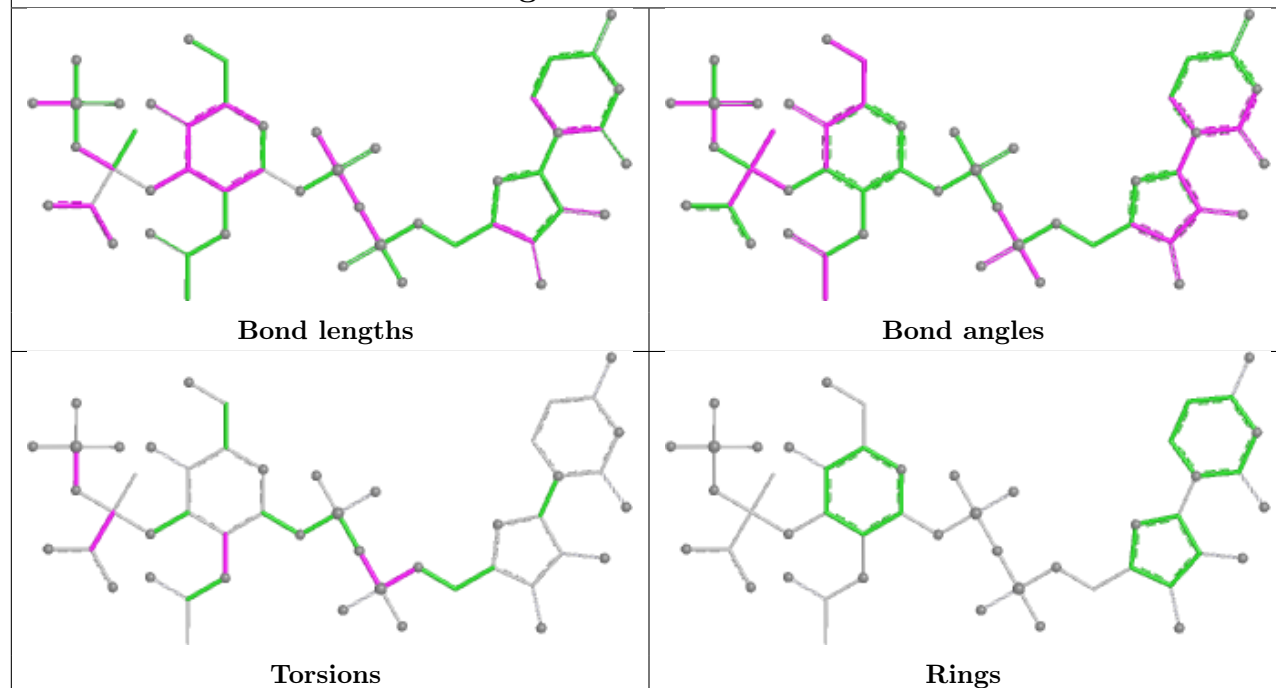
Ligand UDA D 1453



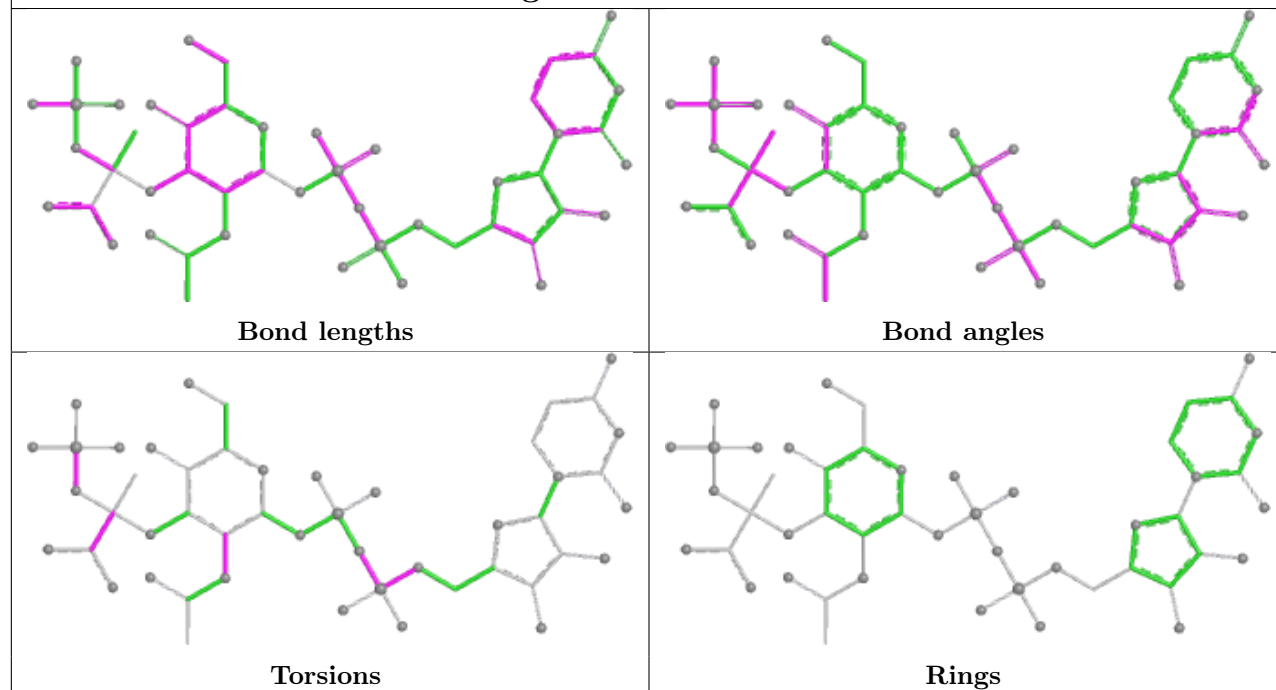
Ligand UDA K 1460



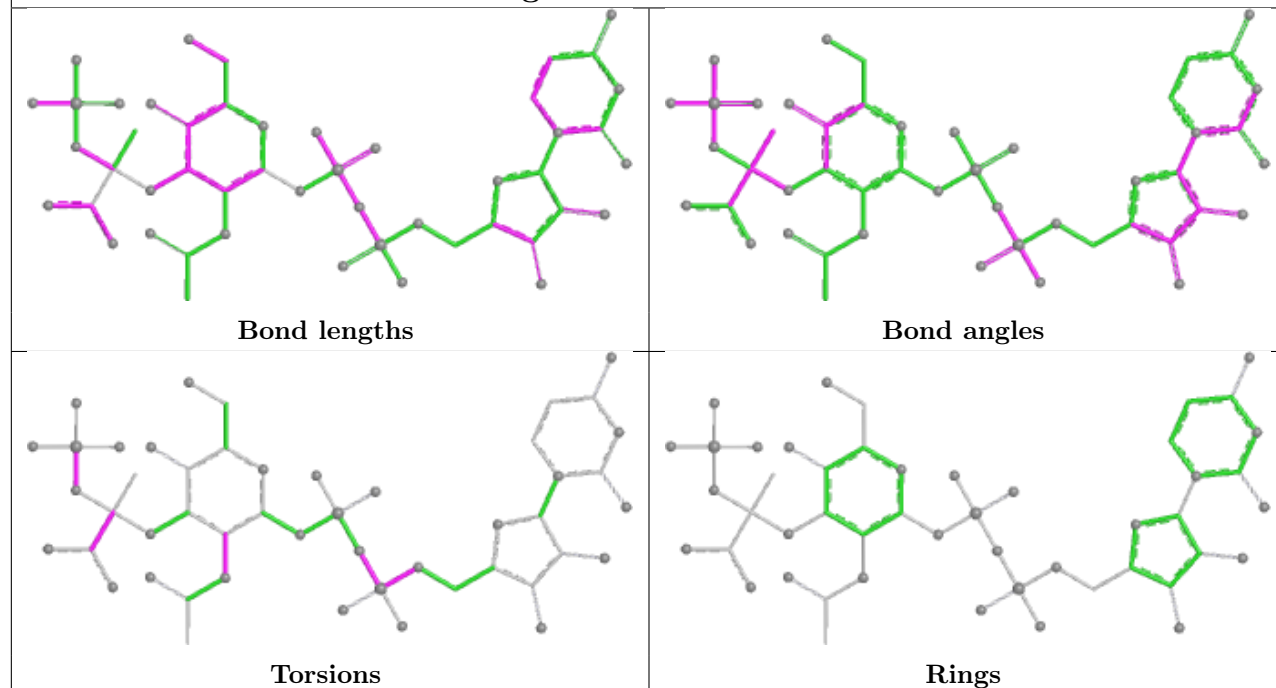
Ligand UDA G 1456



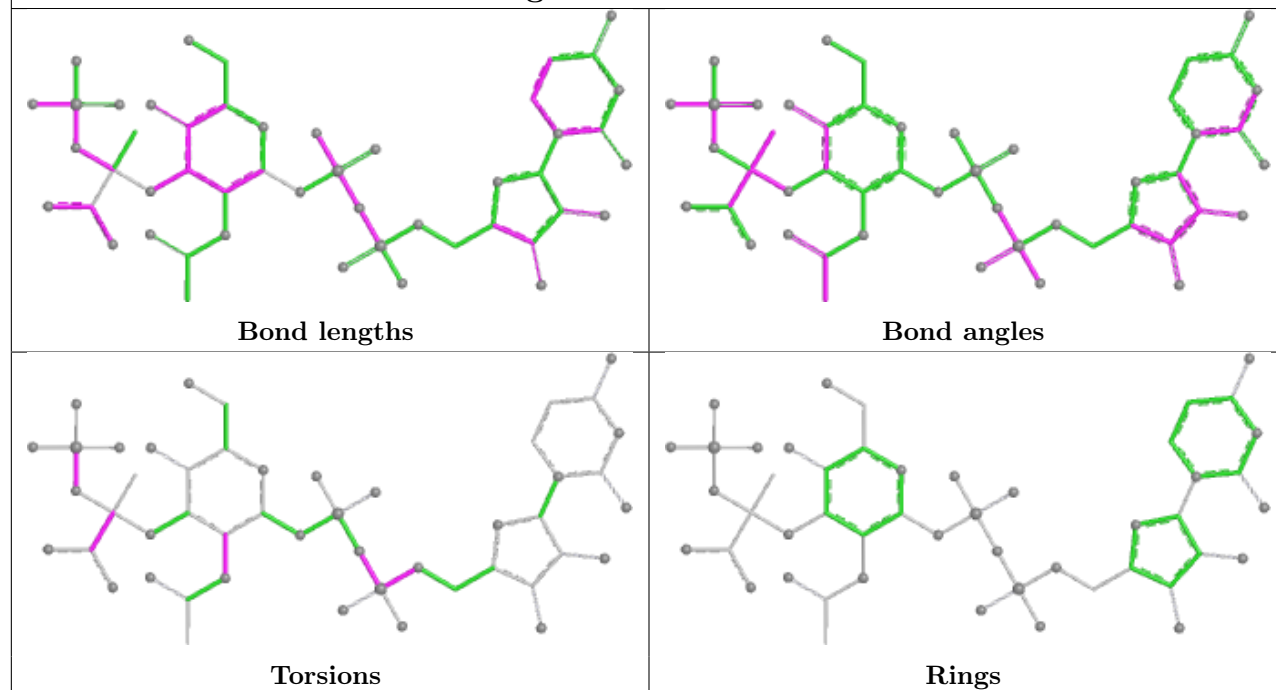
Ligand UDA Z 1465



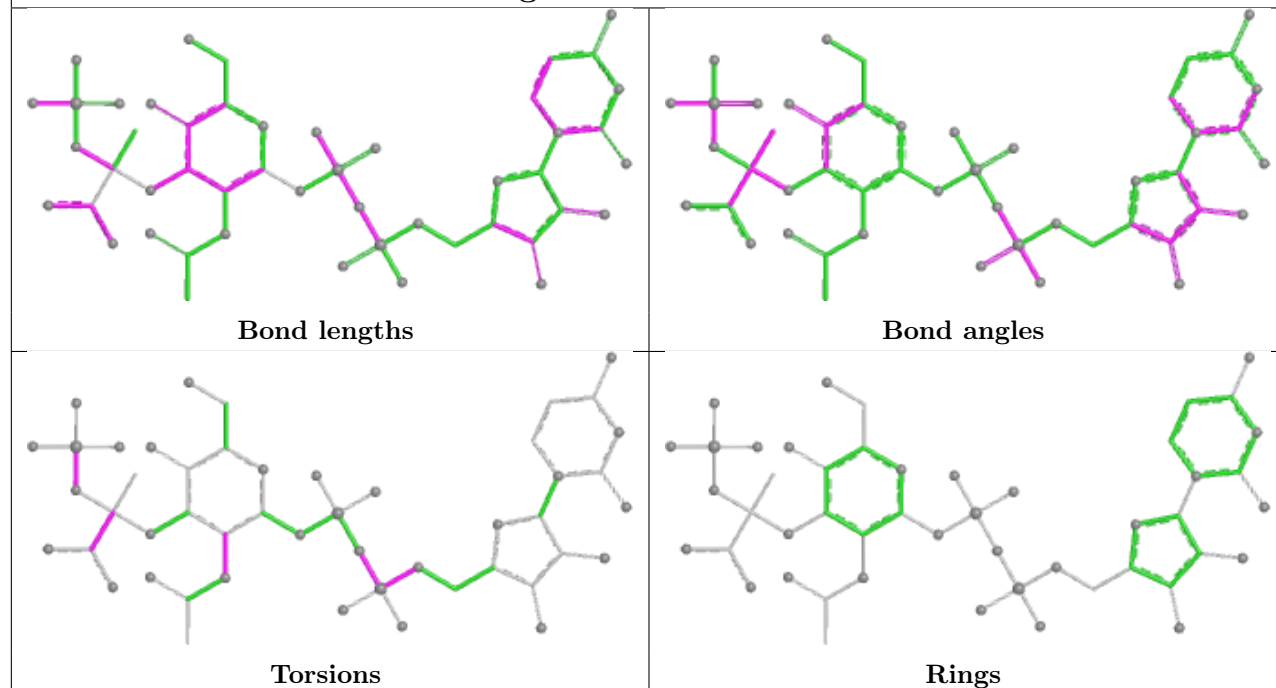
Ligand UDA L 1461



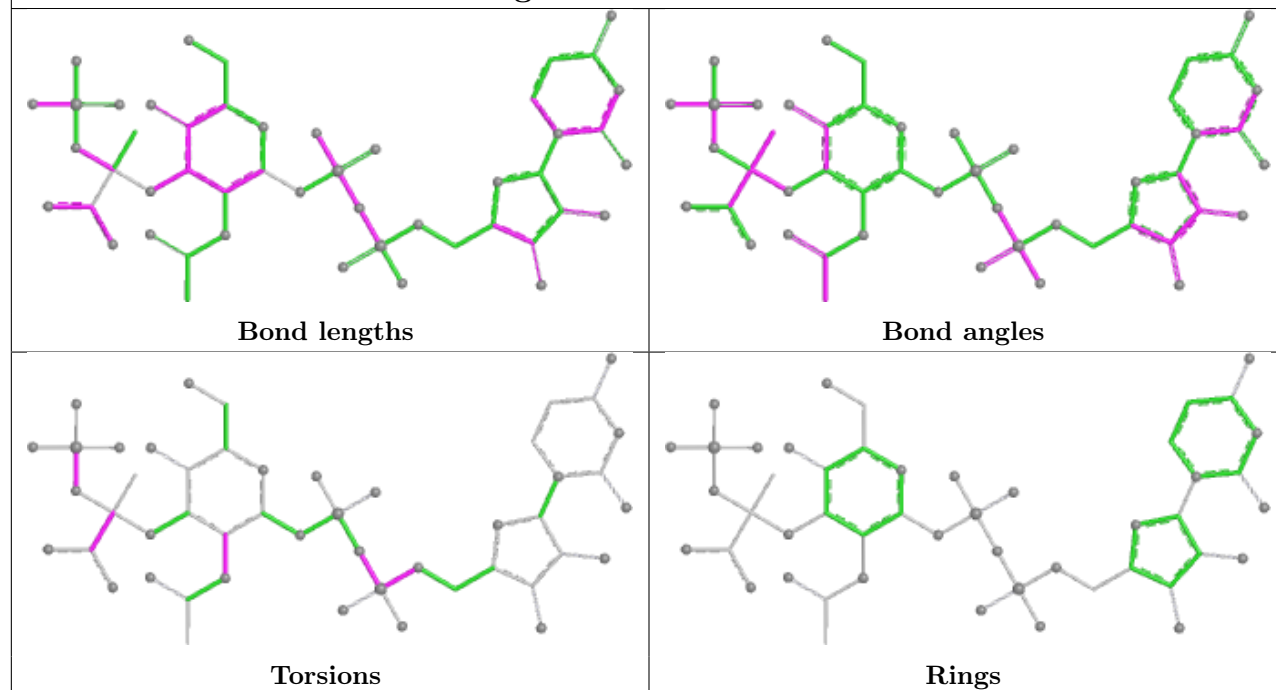
Ligand UDA I 1458



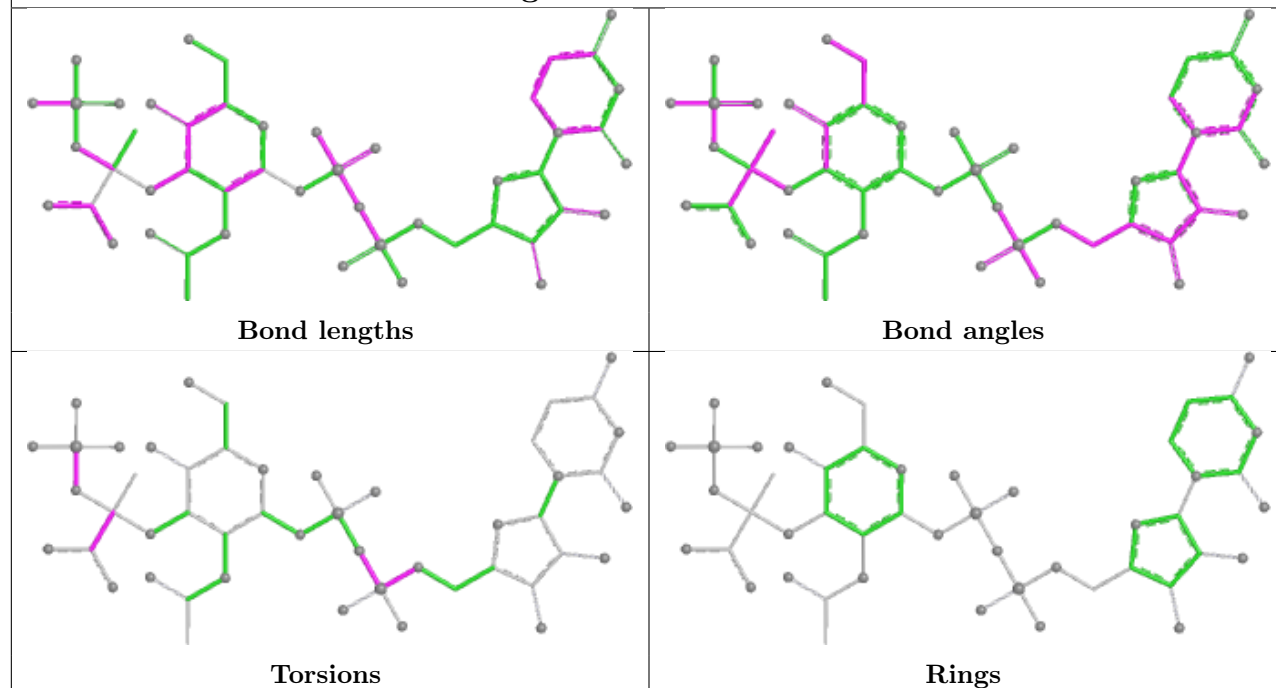
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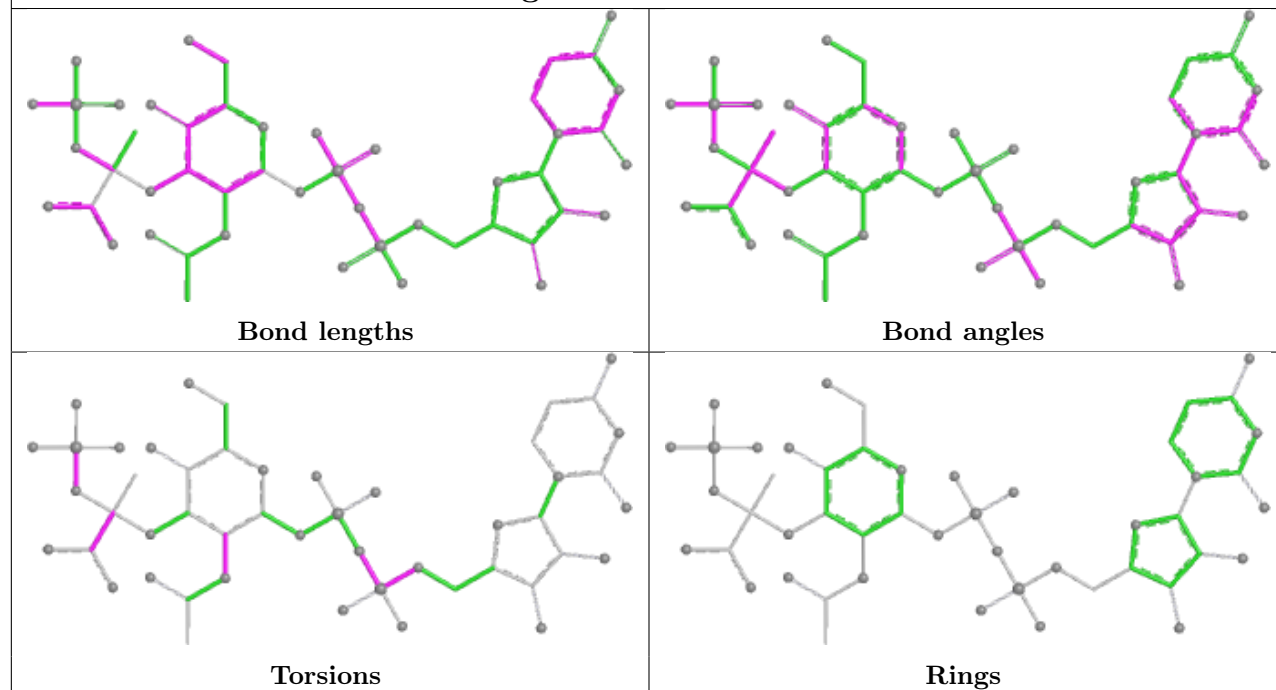
Ligand UDA W 1462

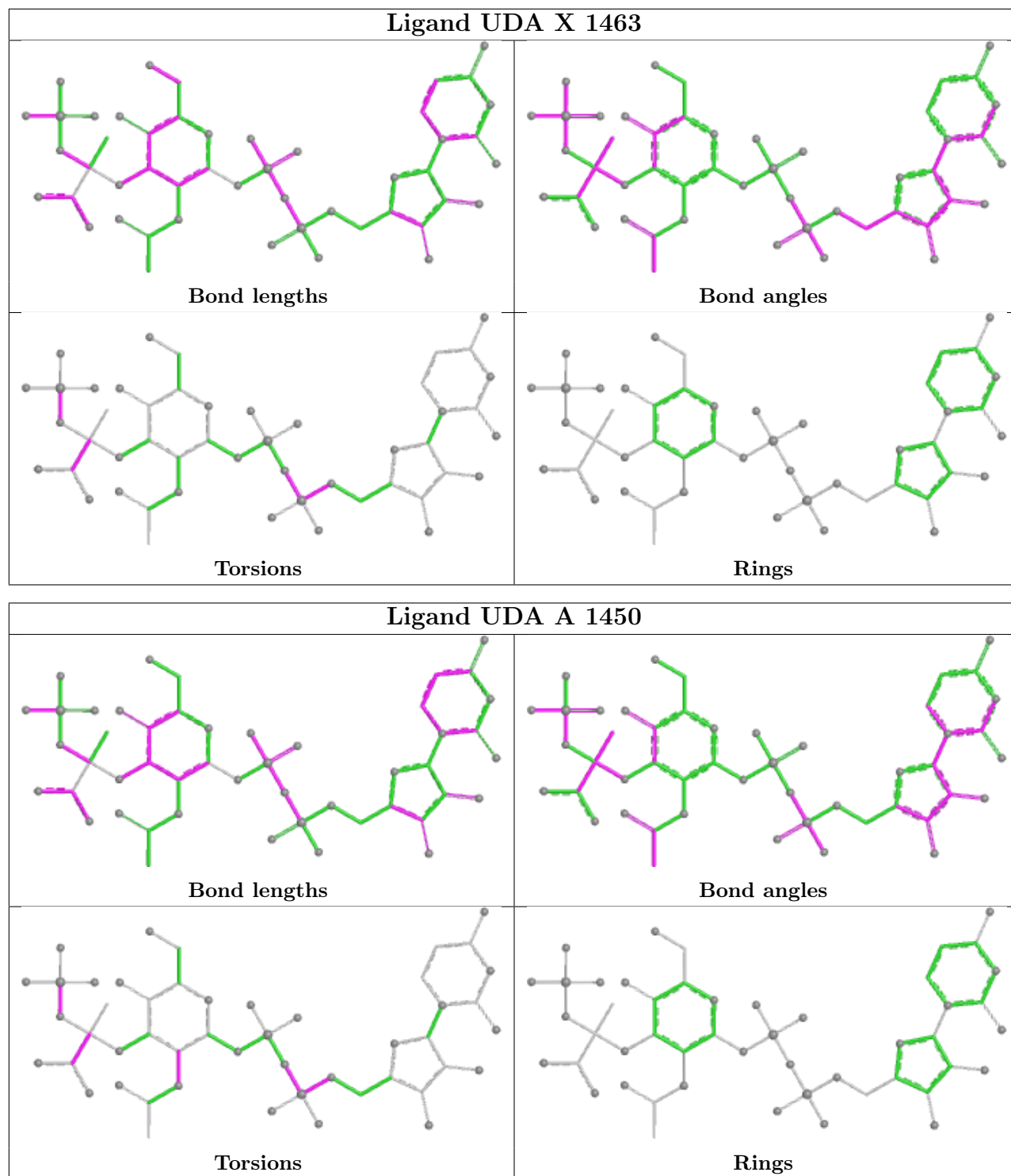


Ligand UDA E 1454



Ligand UDA F 1455





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	418/419 (99%)	-0.36	1 (0%) 91 90	18, 35, 58, 99	0
1	B	418/419 (99%)	-0.42	1 (0%) 91 90	20, 34, 52, 107	0
1	C	418/419 (99%)	-0.55	1 (0%) 91 90	19, 31, 47, 93	0
1	D	418/419 (99%)	-0.53	2 (0%) 87 85	18, 32, 50, 109	0
1	E	418/419 (99%)	-0.50	0 100 100	18, 32, 50, 93	0
1	F	418/419 (99%)	-0.43	0 100 100	20, 34, 50, 93	0
1	G	418/419 (99%)	-0.52	0 100 100	18, 31, 47, 86	0
1	H	418/419 (99%)	-0.49	0 100 100	18, 34, 53, 104	0
1	I	418/419 (99%)	-0.43	0 100 100	20, 34, 52, 105	0
1	J	418/419 (99%)	-0.38	1 (0%) 91 90	22, 37, 56, 103	0
1	K	418/419 (99%)	-0.38	2 (0%) 87 85	20, 36, 53, 102	0
1	L	418/419 (99%)	-0.33	0 100 100	22, 37, 58, 92	0
1	W	418/419 (99%)	-0.36	1 (0%) 91 90	22, 35, 54, 96	0
1	X	418/419 (99%)	-0.25	0 100 100	22, 38, 61, 99	0
1	Y	418/419 (99%)	-0.26	2 (0%) 87 85	23, 37, 54, 99	0
1	Z	418/419 (99%)	-0.27	0 100 100	22, 39, 61, 89	0
All	All	6688/6704 (99%)	-0.40	11 (0%) 91 90	18, 35, 54, 109	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	418	GLY	3.3
1	C	418	GLY	3.0
1	D	419	GLU	2.9
1	K	61	GLY	2.8
1	Y	61	GLY	2.7

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

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
1	IAS	A	67	8/9	0.79	0.10	45,47,49,51	0
1	IAS	W	67	8/9	0.79	0.12	33,38,42,42	0
1	IAS	K	67	8/9	0.80	0.10	43,48,51,56	0
1	IAS	Y	67	8/9	0.80	0.12	45,46,50,55	0
1	IAS	I	67	8/9	0.81	0.11	37,40,41,44	0
1	IAS	Z	67	8/9	0.83	0.08	47,48,51,53	0
1	IAS	E	67	8/9	0.85	0.14	40,44,47,49	0
1	IAS	B	67	8/9	0.86	0.08	40,43,47,50	0
1	IAS	J	67	8/9	0.87	0.10	43,46,48,50	0
1	IAS	L	67	8/9	0.90	0.08	44,46,48,52	0
1	IAS	C	67	8/9	0.90	0.08	31,35,37,37	0
1	IAS	H	67	8/9	0.91	0.09	30,41,46,51	0
1	IAS	F	67	8/9	0.92	0.07	37,41,44,46	0
1	IAS	G	67	8/9	0.92	0.08	30,33,39,39	0
1	IAS	D	67	8/9	0.93	0.07	32,40,44,45	0
1	IAS	X	67	8/9	0.94	0.06	45,46,50,52	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	EDO	F	1475	4/4	0.69	0.16	32,35,37,38	0
3	EDO	D	1473	4/4	0.78	0.16	31,32,38,41	0
3	EDO	A	1470	4/4	0.87	0.15	36,36,42,42	0
3	EDO	L	1481	4/4	0.87	0.11	42,42,50,53	0
3	EDO	Z	1485	4/4	0.89	0.10	39,40,43,46	0
3	EDO	X	1483	4/4	0.92	0.08	41,45,45,47	0

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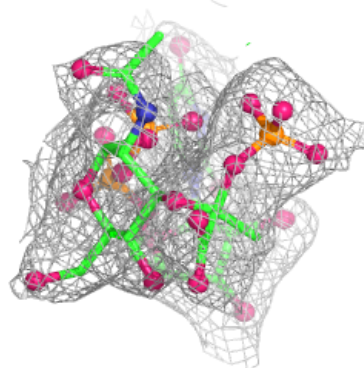
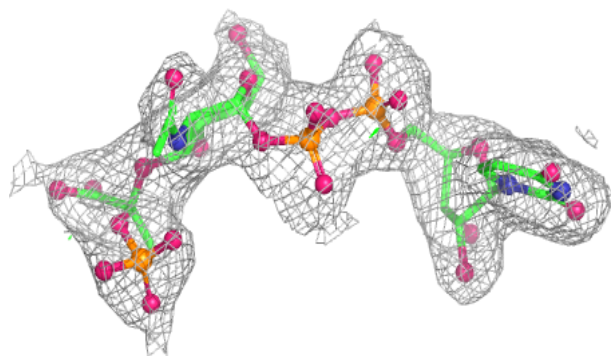
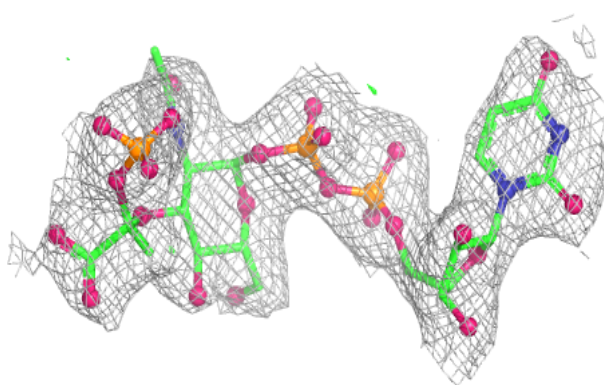
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	W	1482	4/4	0.92	0.08	28,30,34,38	0
3	EDO	B	1471	4/4	0.93	0.10	25,32,37,44	0
3	EDO	C	1472	4/4	0.94	0.08	23,28,32,38	0
3	EDO	E	1474	4/4	0.95	0.10	33,36,39,41	0
2	UDA	Z	1465	49/49	0.95	0.08	25,38,61,66	0
3	EDO	H	1477	4/4	0.95	0.07	26,28,29,31	0
2	UDA	A	1450	49/49	0.95	0.08	20,32,56,63	0
2	UDA	J	1459	49/49	0.95	0.08	27,36,57,61	0
2	UDA	W	1462	49/49	0.95	0.08	19,40,51,56	0
3	EDO	Y	1484	4/4	0.95	0.09	29,29,32,39	0
2	UDA	X	1463	49/49	0.95	0.08	30,41,57,60	0
2	UDA	G	1456	49/49	0.96	0.07	11,30,59,65	0
2	UDA	H	1457	49/49	0.96	0.07	16,33,53,57	0
2	UDA	I	1458	49/49	0.96	0.07	16,35,51,55	0
2	UDA	B	1451	49/49	0.96	0.07	23,34,54,57	0
2	UDA	K	1460	49/49	0.96	0.07	24,30,54,58	0
3	EDO	G	1476	4/4	0.96	0.07	23,26,30,38	0
2	UDA	L	1461	49/49	0.96	0.07	24,38,57,58	0
3	EDO	K	1480	4/4	0.96	0.06	28,30,33,38	0
2	UDA	C	1452	49/49	0.96	0.07	22,32,56,61	0
2	UDA	D	1453	49/49	0.96	0.07	24,32,45,50	0
2	UDA	Y	1464	49/49	0.96	0.07	22,30,53,55	0
2	UDA	E	1454	49/49	0.96	0.08	17,27,53,57	0
2	UDA	F	1455	49/49	0.96	0.07	26,32,49,52	0
3	EDO	J	1479	4/4	0.97	0.06	28,30,31,32	0
3	EDO	I	1478	4/4	0.98	0.04	30,31,34,40	0

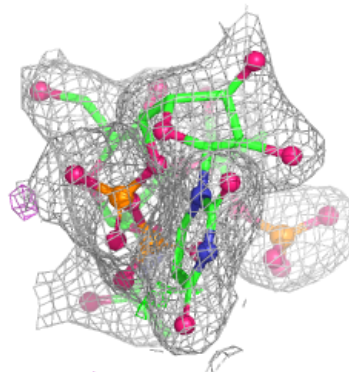
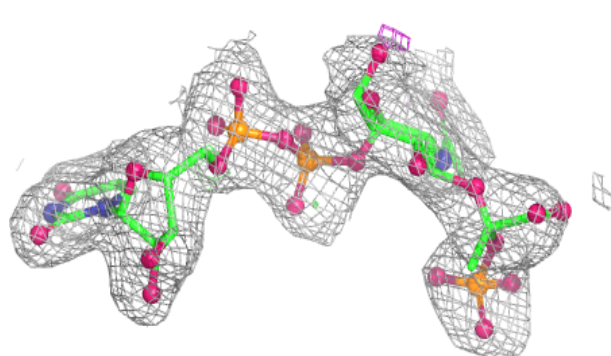
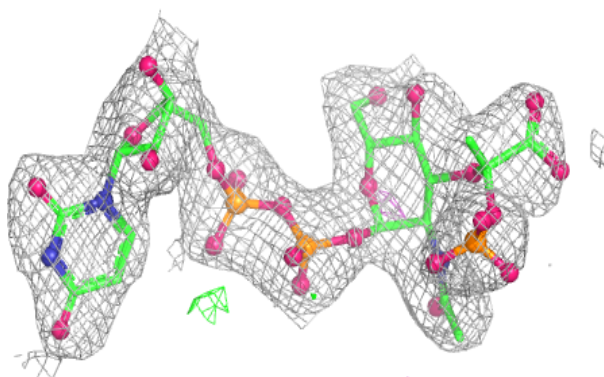
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDA Z 1465:

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

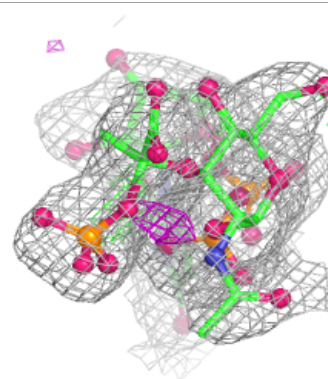
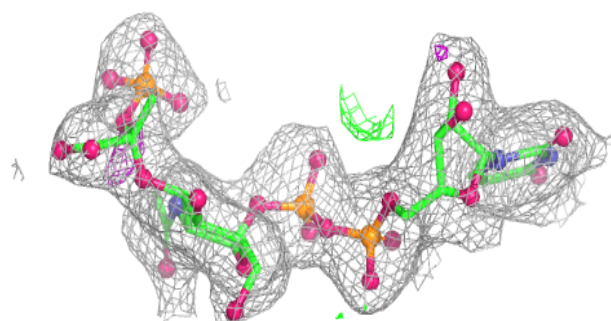
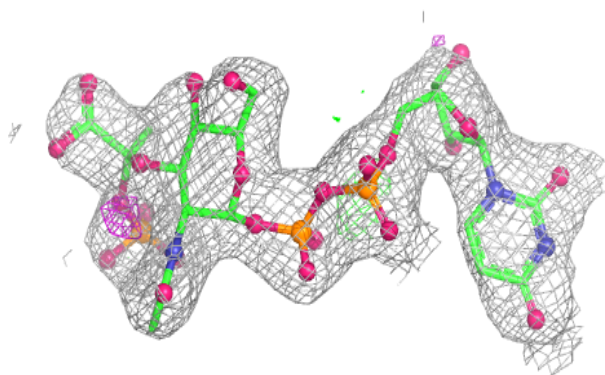
**Electron density around UDA A 1450:**

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

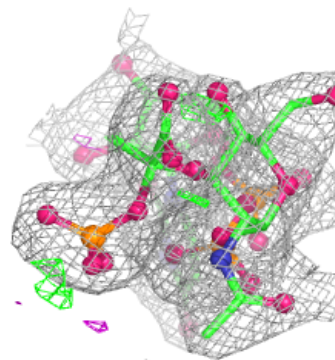
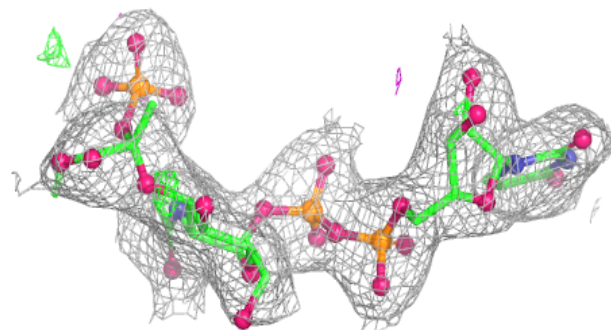
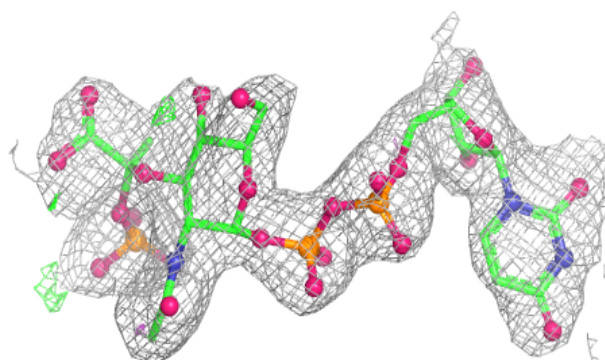


Electron density around UDA J 1459:

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and green (positive)

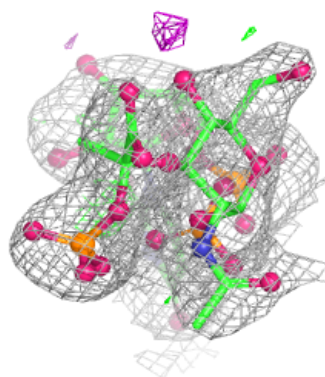
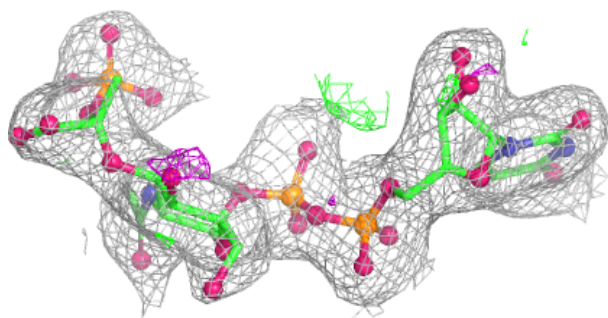
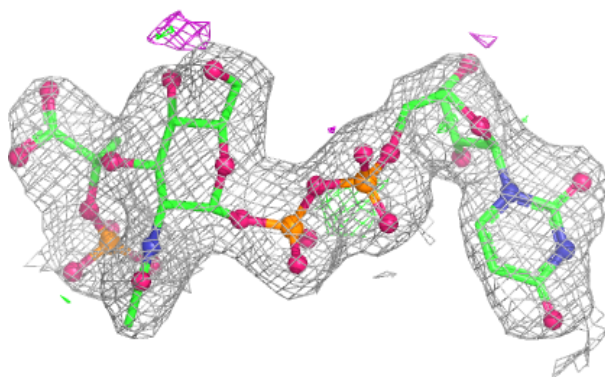
**Electron density around UDA W 1462:**

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and green (positive)

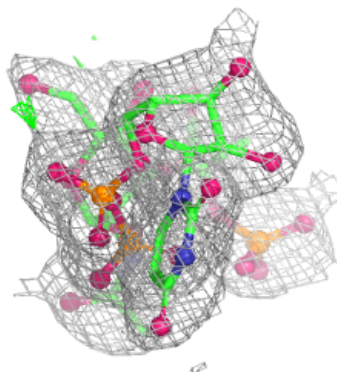
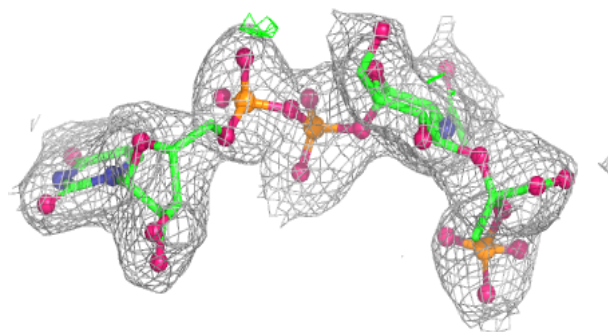
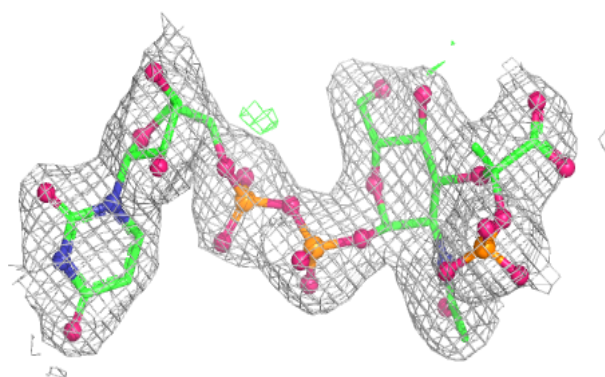


Electron density around UDA X 1463:

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

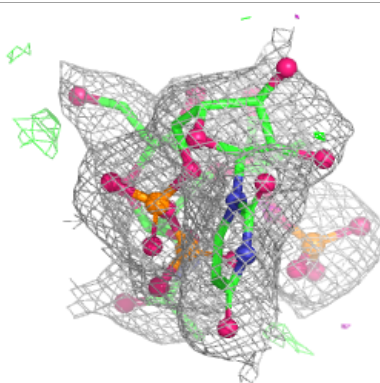
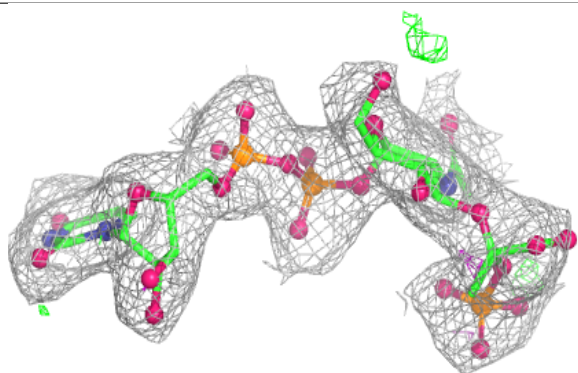
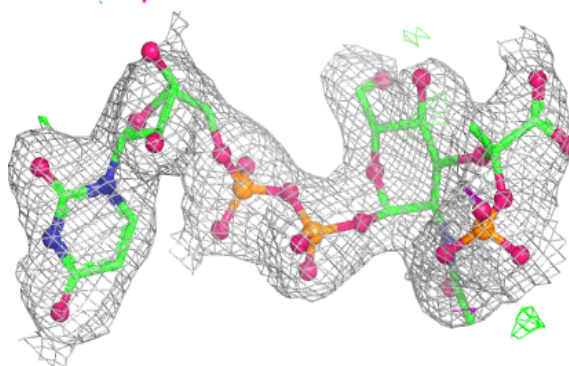
**Electron density around UDA G 1456:**

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and green (positive)

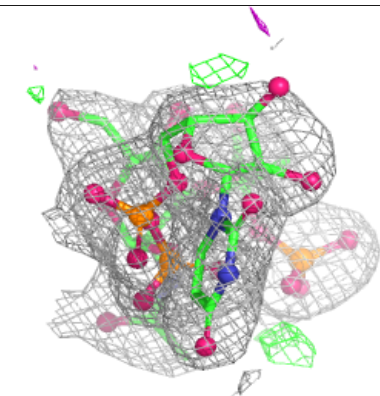
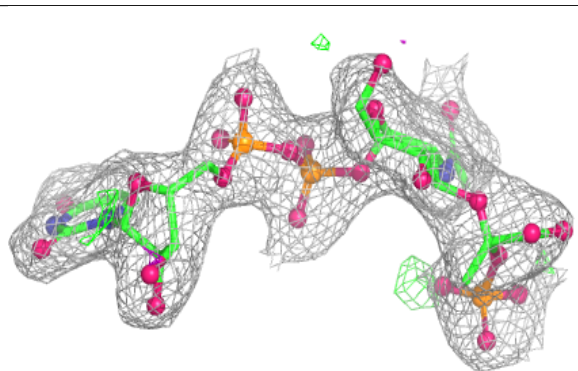
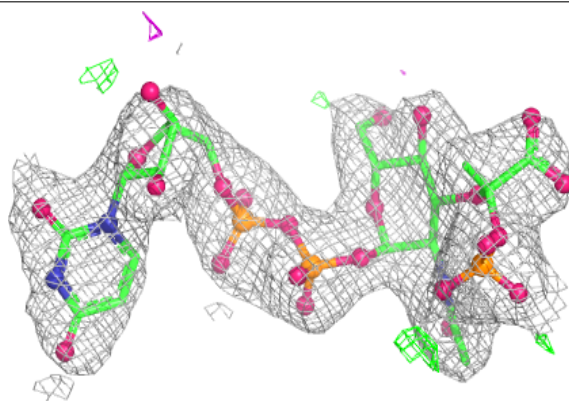


Electron density around UDA H 1457:

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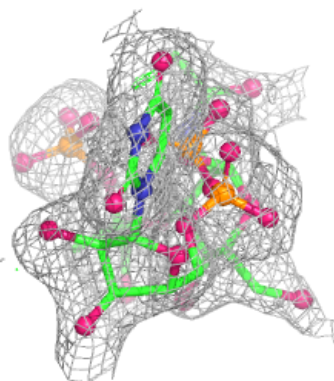
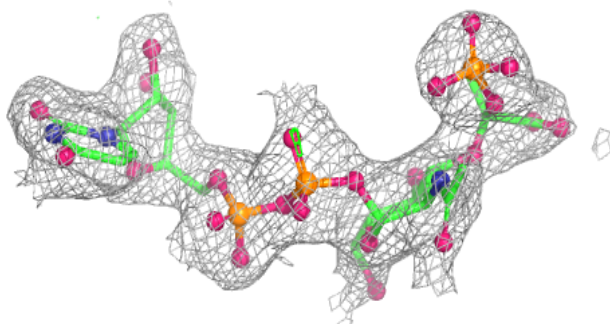
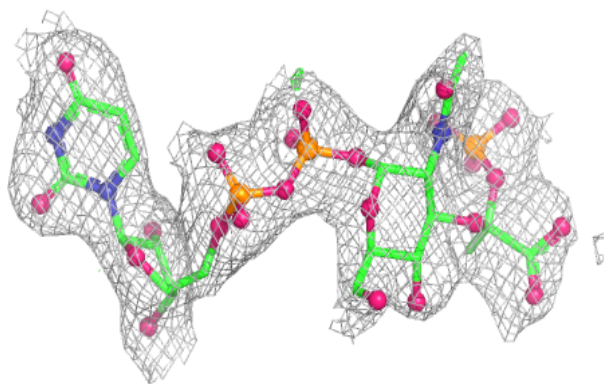
**Electron density around UDA I 1458:**

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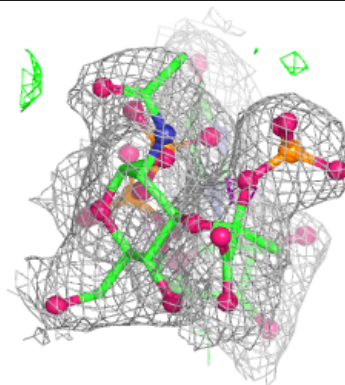
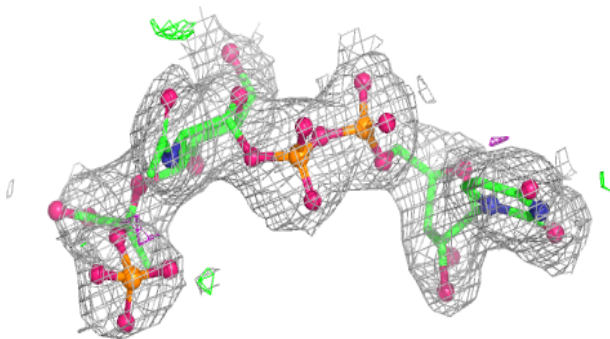
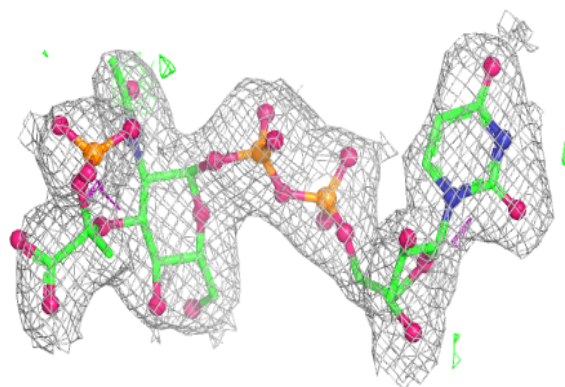


Electron density around UDA B 1451:

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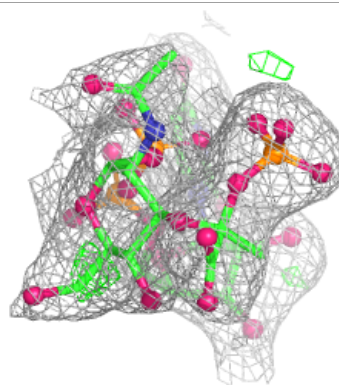
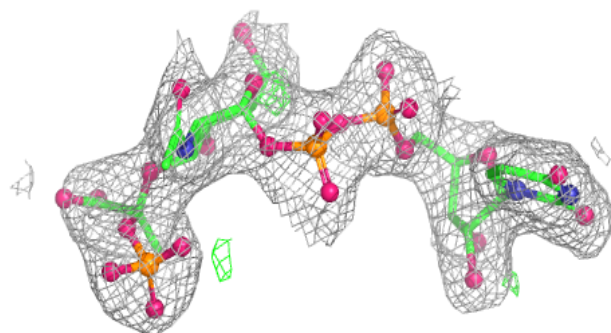
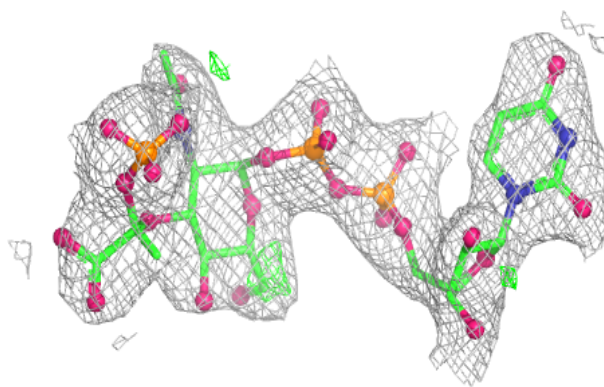
**Electron density around UDA K 1460:**

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

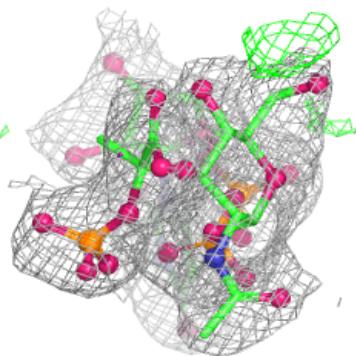
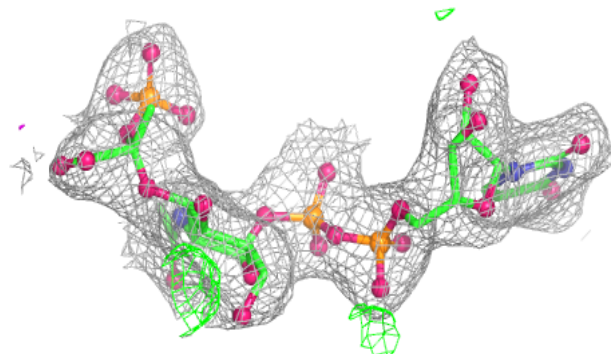
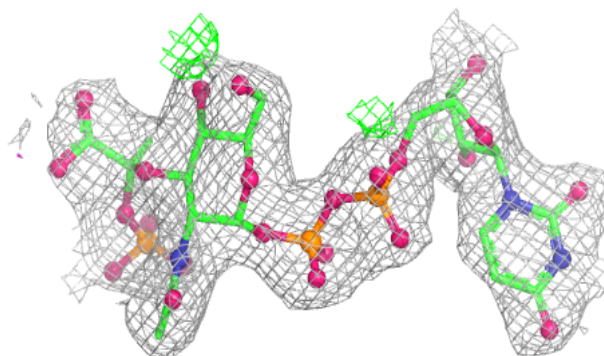


Electron density around UDA L 1461:

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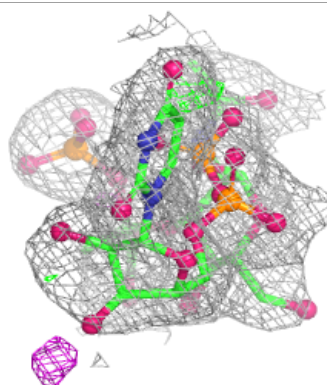
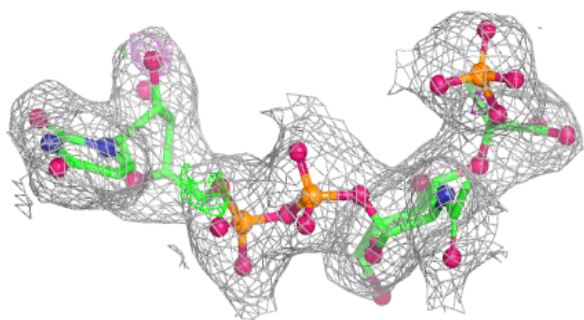
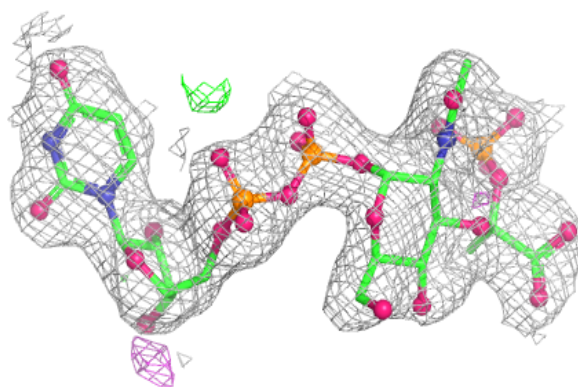
**Electron density around UDA C 1452:**

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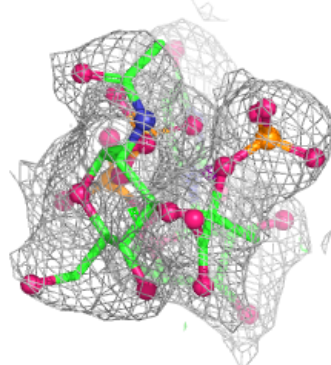
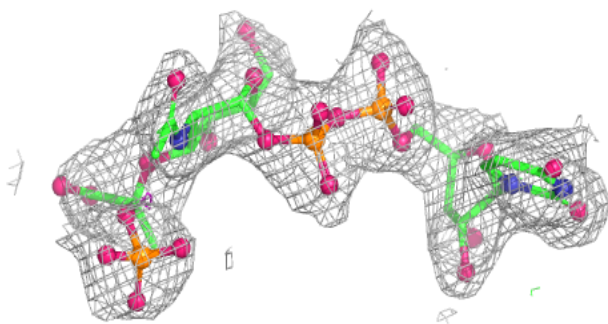
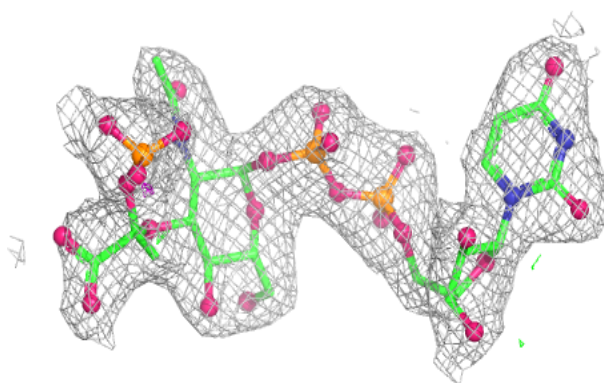


Electron density around UDA D 1453:

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and green (positive)

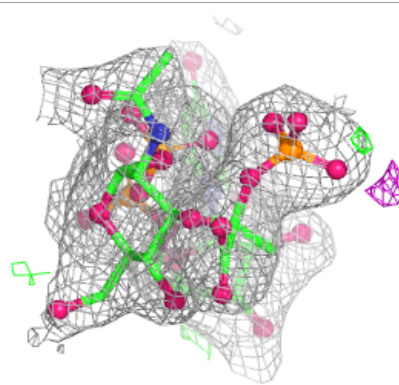
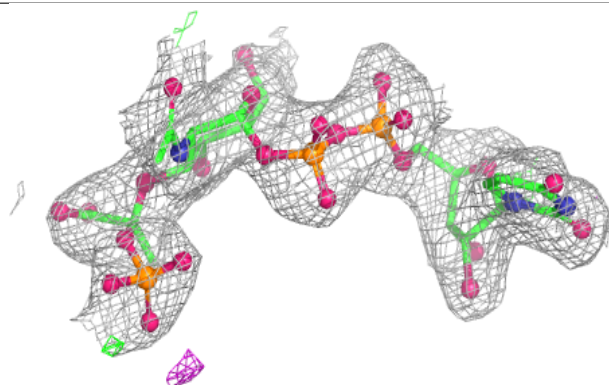
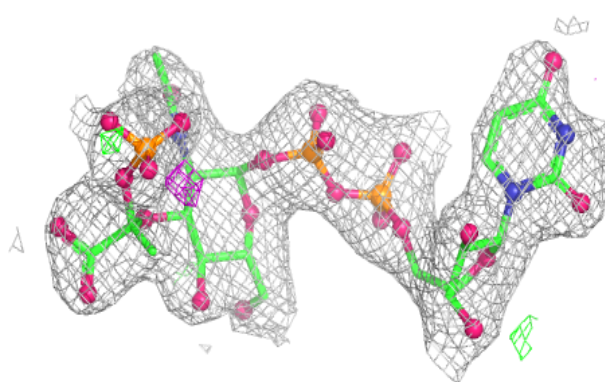
**Electron density around UDA Y 1464:**

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

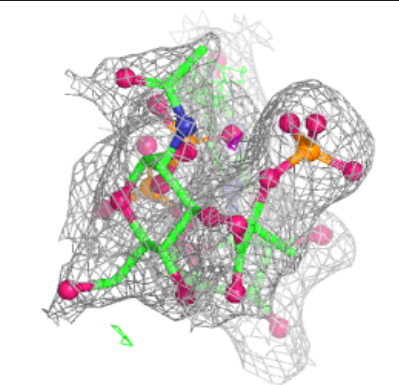
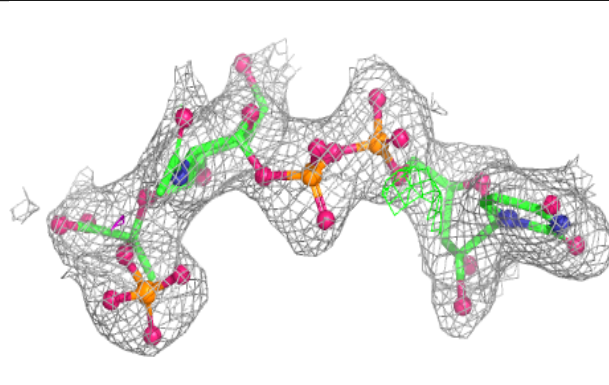
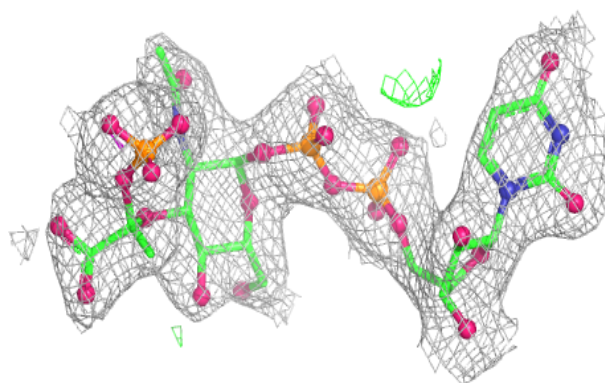


Electron density around UDA E 1454:

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

**Electron density around UDA F 1455:**

$2mF_o - DF_c$ (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.