



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 30, 2025 – 04:15 am BST

PDB ID : 9ESL / pdb_00009esl
Title : CDK2-cyclin A in complex with FragLite 29
Authors : Hope, I.; Martin, M.P.; Waring, M.J.; Noble, M.E.M.; Endicott, J.A.; Tatum, N.J.
Deposited on : 2024-03-26
Resolution : 2.39 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 : 4.02b-467
Mogul : ?? (???), CSD ??CSD?? (????)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

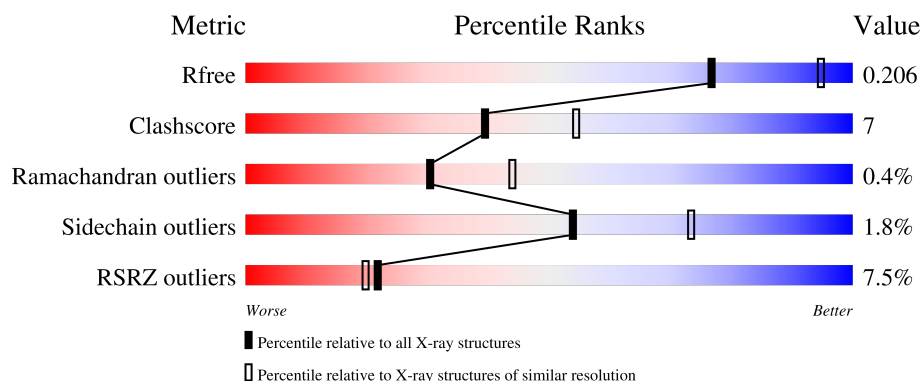
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	302	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>
1	C	302	<div> <div>7%</div> <div> <div></div> <div>76%</div> <div>11%</div> <div>.</div> <div>11%</div> </div> </div>
2	B	268	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>.</div> </div> </div>
2	D	268	<div> <div>13%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	V3U	A	303	-	-	X	-
3	V3U	B	701[A]	-	-	-	X
3	V3U	B	701[B]	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9290 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	P	S	0	2	0
			2432	1575	416	432	1	8			
1	C	269	Total	C	N	O	P	S	0	1	0
			2168	1404	372	384	1	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P24941
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-3	GLY	-	expression tag	UNP P24941
C	-2	PRO	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	262	Total	C	N	O	S	0	1	0
			2118	1370	345	393	10			
2	D	262	Total	C	N	O	S	0	1	0
			2118	1370	345	393	10			

There are 14 discrepancies between the modelled and reference sequences:

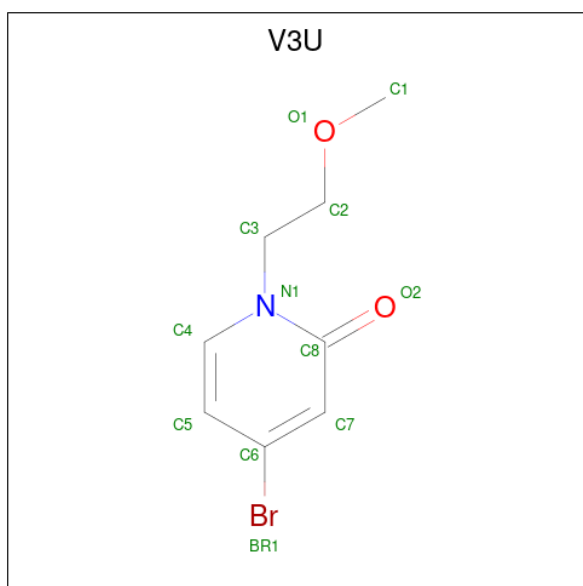
Chain	Residue	Modelled	Actual	Comment	Reference
B	171	GLY	-	expression tag	UNP P30274
B	433	HIS	-	expression tag	UNP P30274
B	434	HIS	-	expression tag	UNP P30274
B	435	HIS	-	expression tag	UNP P30274

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Chain	Residue	Modelled	Actual	Comment	Reference
B	436	HIS	-	expression tag	UNP P30274
B	437	HIS	-	expression tag	UNP P30274
B	438	HIS	-	expression tag	UNP P30274
D	171	GLY	-	expression tag	UNP P30274
D	433	HIS	-	expression tag	UNP P30274
D	434	HIS	-	expression tag	UNP P30274
D	435	HIS	-	expression tag	UNP P30274
D	436	HIS	-	expression tag	UNP P30274
D	437	HIS	-	expression tag	UNP P30274
D	438	HIS	-	expression tag	UNP P30274

- Molecule 3 is 4-bromanyl-1-(2-methoxyethyl)pyridin-2-one (CCD ID: V3U) (formula: $C_8H_{10}BrNO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			12	1	8	1	2		
3	A	1	Total	Br	C	N	O	0	0
			12	1	8	1	2		
3	A	1	Total	Br	C	N	O	0	0
			12	1	8	1	2		
3	B	1	Total	Br	C	N	O	0	1
			24	2	16	2	4		
3	C	1	Total	Br	C	N	O	0	1
			24	2	16	2	4		
3	C	1	Total	Br	C	N	O	0	0
			12	1	8	1	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	Br	C	N	O	0	0
			12	1	8	1	2		

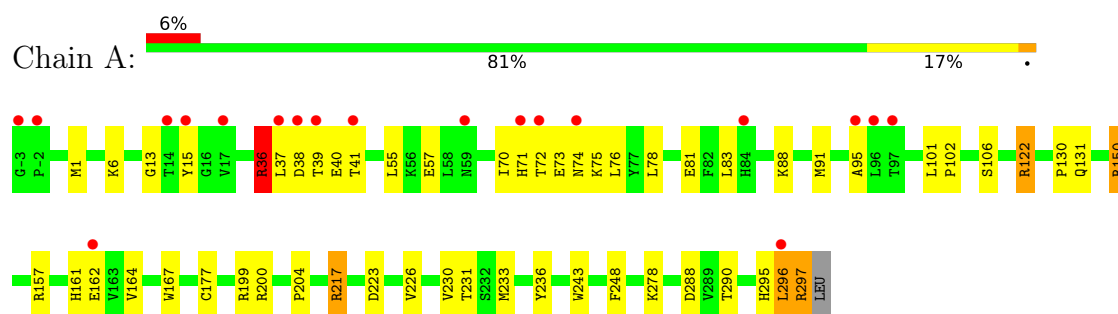
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		
4	B	122	Total	O	0	0
			122	122		
4	C	52	Total	O	0	0
			52	52		
4	D	43	Total	O	0	0
			43	43		

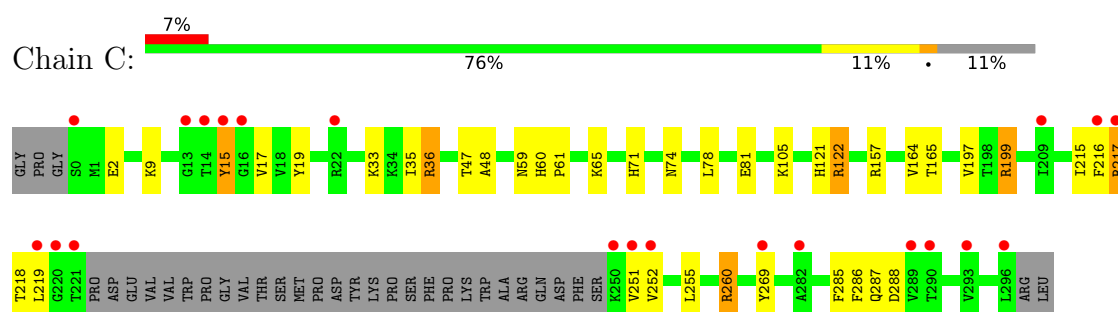
3 Residue-property plots

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.

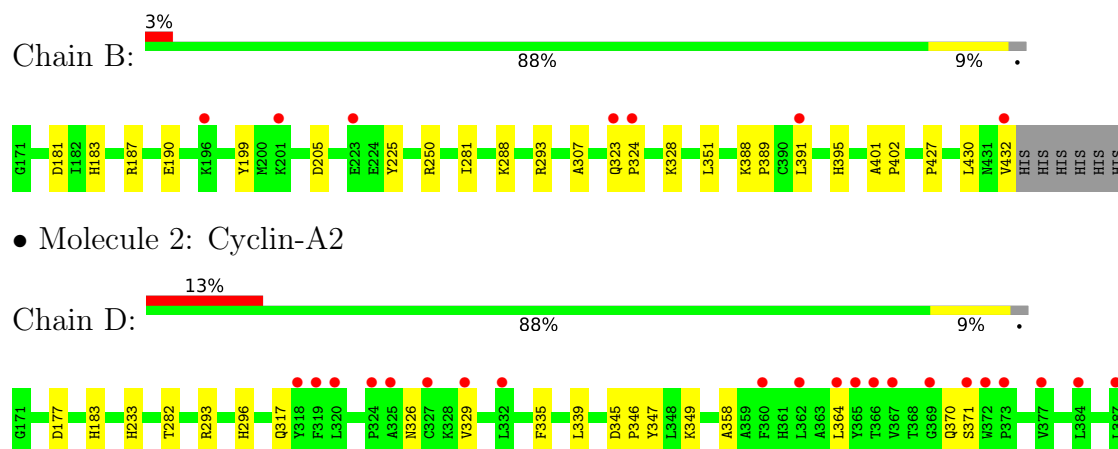
• Molecule 1: Cyclin-dependent kinase 2



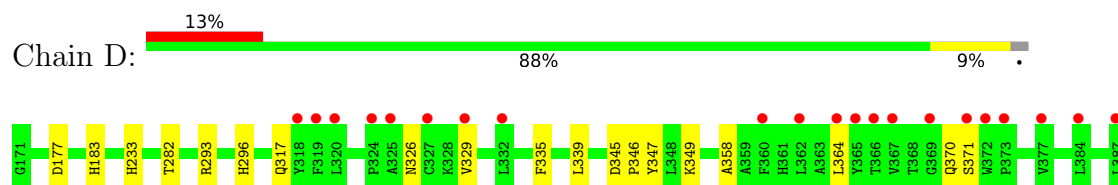
• Molecule 1: Cyclin-dependent kinase 2

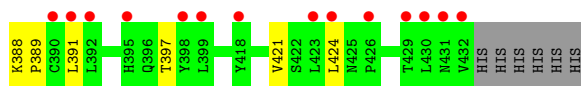


• Molecule 2: Cyclin-A2



• Molecule 2: Cyclin-A2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.13Å 134.21Å 147.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.57 – 2.39 99.38 – 2.39	Depositor EDS
% Data completeness (in resolution range)	96.5 (99.57-2.39) 96.5 (99.38-2.39)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.217 , 0.220 0.204 , 0.206	Depositor DCC
R_{free} test set	2921 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9290	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: V3U, TPO

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	0/2484	0.78	0/3370
1	C	0.43	0/2205	0.78	0/2984
2	B	0.45	0/2168	0.76	0/2948
2	D	0.41	0/2168	0.72	0/2948
All	All	0.44	0/9025	0.76	0/12250

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	C	0	3
2	B	0	2
2	D	0	1
All	All	0	13

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	ARG	Sidechain
1	A	150	ARG	Sidechain
1	A	157	ARG	Sidechain
1	A	200	ARG	Sidechain
1	A	36	ARG	Sidechain

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	2432	0	2467	52	0
1	C	2168	0	2228	33	0
2	B	2118	0	2131	14	0
2	D	2118	0	2131	23	0
3	A	36	0	0	7	0
3	B	24	0	0	0	0
3	C	36	0	0	3	0
3	D	12	0	0	2	0
4	A	129	0	0	1	0
4	B	122	0	0	1	0
4	C	52	0	0	2	0
4	D	43	0	0	1	0
All	All	9290	0	8957	119	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 7.

The worst 5 of 119 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:A:1:MET:CE	1:A:70:ILE:HD13	1.75	1.17
1:A:6:LYS:HE3	3:A:303:V3U:BR1	2.09	1.07
1:C:9:LYS:HE3	1:C:17:VAL:HG23	1.38	1.05
1:C:59:ASN:ND2	1:C:65:LYS:HE3	1.72	1.03
1:A:1:MET:HE2	1:A:70:ILE:HD13	1.48	0.93

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	300/302 (99%)	293 (98%)	6 (2%)	1 (0%)	37	51
1	C	265/302 (88%)	256 (97%)	6 (2%)	3 (1%)	12	18
2	B	261/268 (97%)	258 (99%)	3 (1%)	0	100	100
2	D	261/268 (97%)	250 (96%)	11 (4%)	0	100	100
All	All	1087/1140 (95%)	1057 (97%)	26 (2%)	4 (0%)	30	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	287	GLN
1	A	164	VAL
1	C	15	TYR
1	C	164	VAL

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	265/264 (100%)	257 (97%)	8 (3%)	36	57
1	C	236/264 (89%)	231 (98%)	5 (2%)	48	69
2	B	235/240 (98%)	233 (99%)	2 (1%)	75	88
2	D	235/240 (98%)	233 (99%)	2 (1%)	75	88
All	All	971/1008 (96%)	954 (98%)	17 (2%)	54	73

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	217	ARG
2	D	371	SER
1	A	297	ARG
2	B	199	TYR

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Mol	Chain	Res	Type
2	B	328	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	71	HIS
1	C	161	HIS
2	D	431	ASN
2	D	317	GLN
2	D	396	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

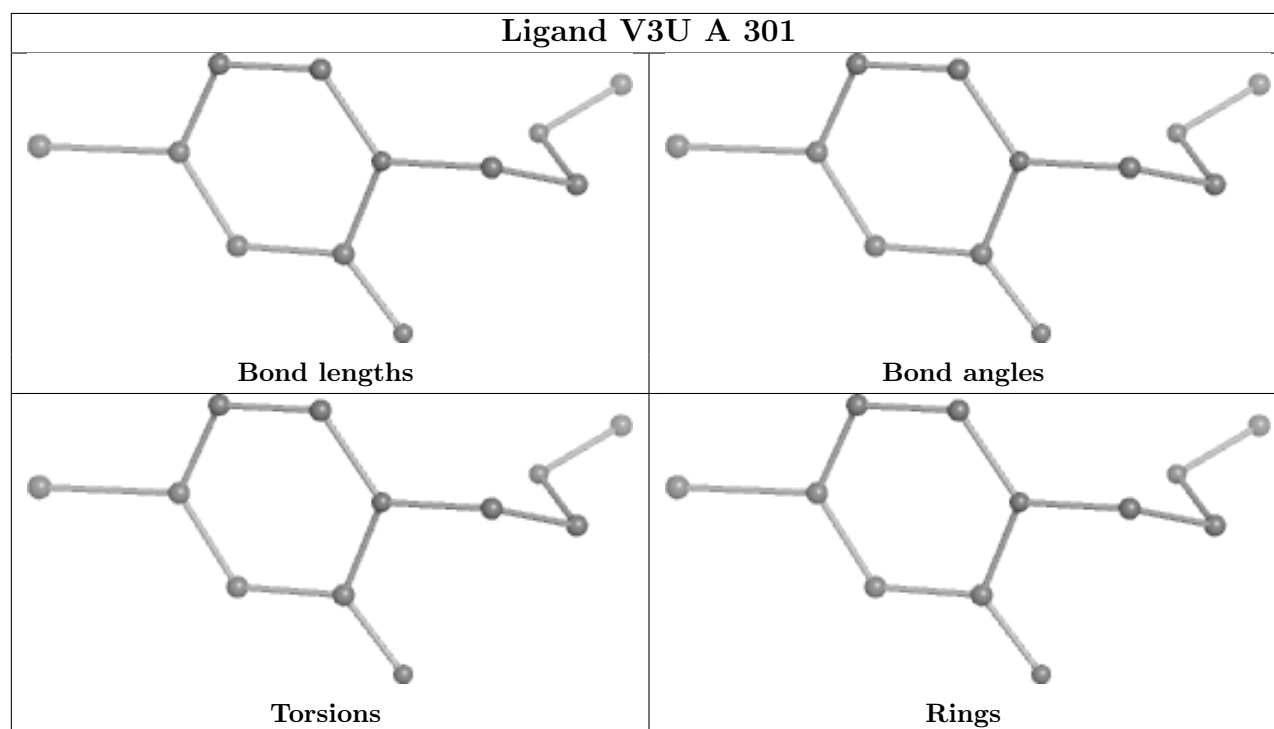
There are no chirality outliers.

There are no torsion outliers.

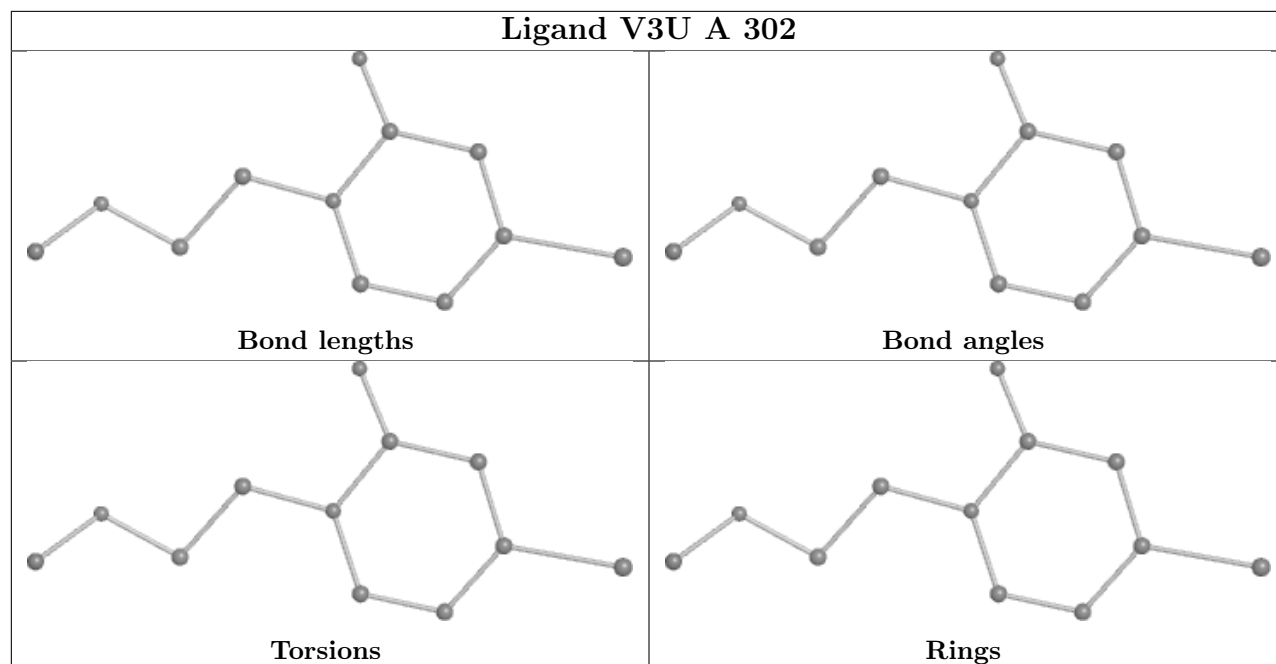
There are no ring outliers.

No monomer is involved in short contacts.

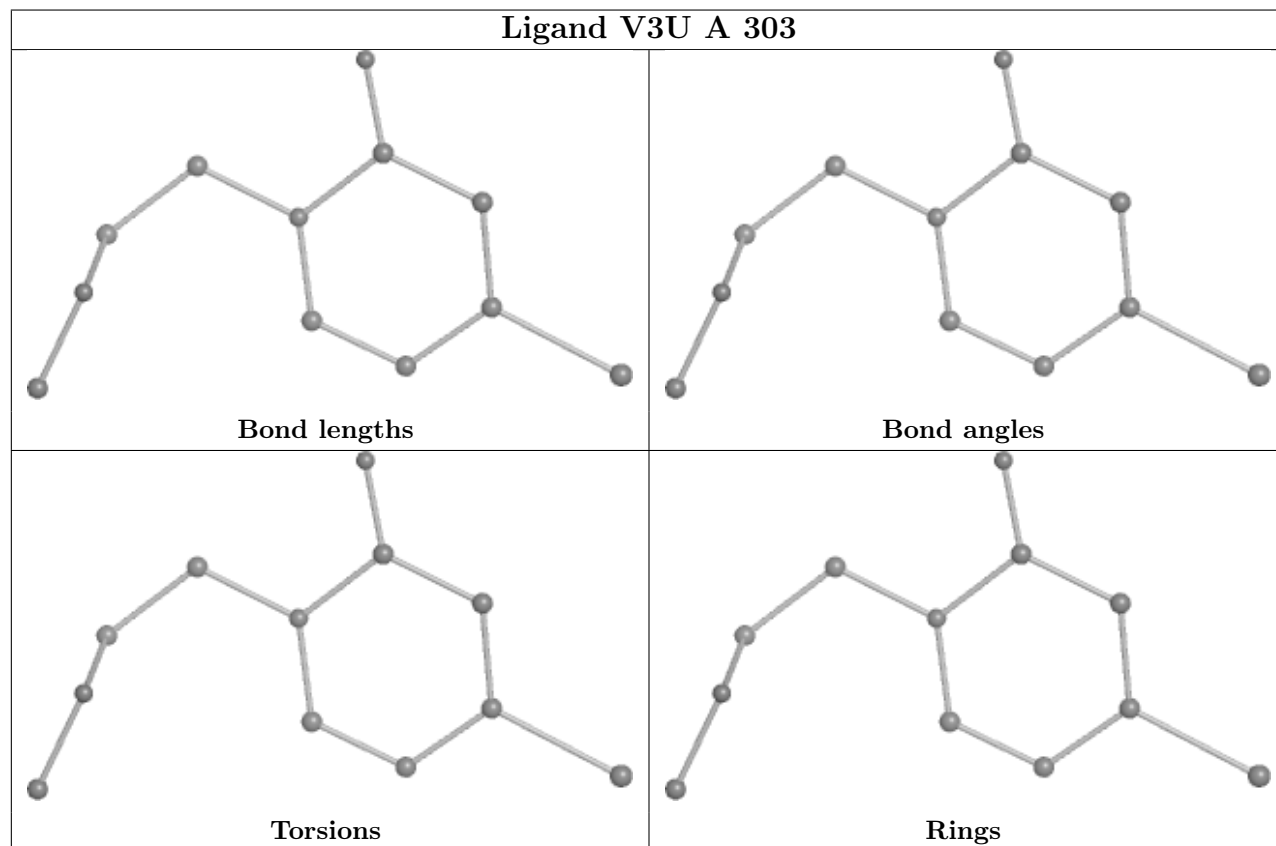
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

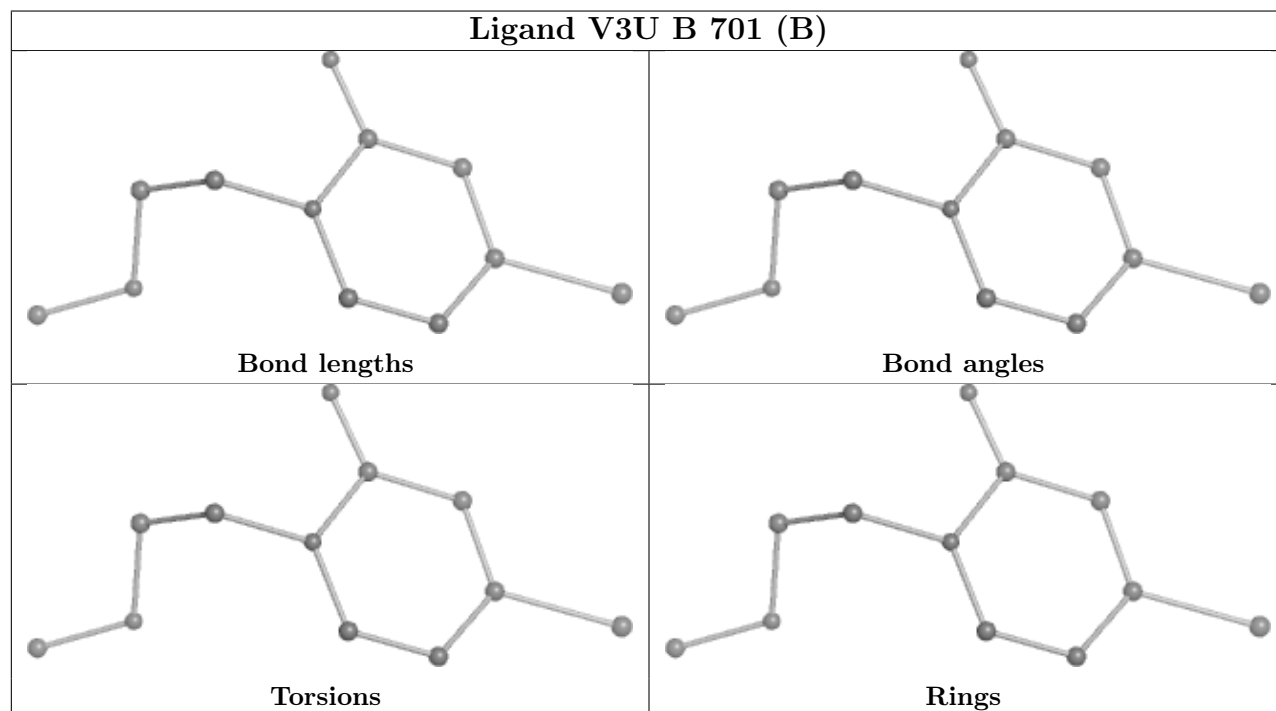
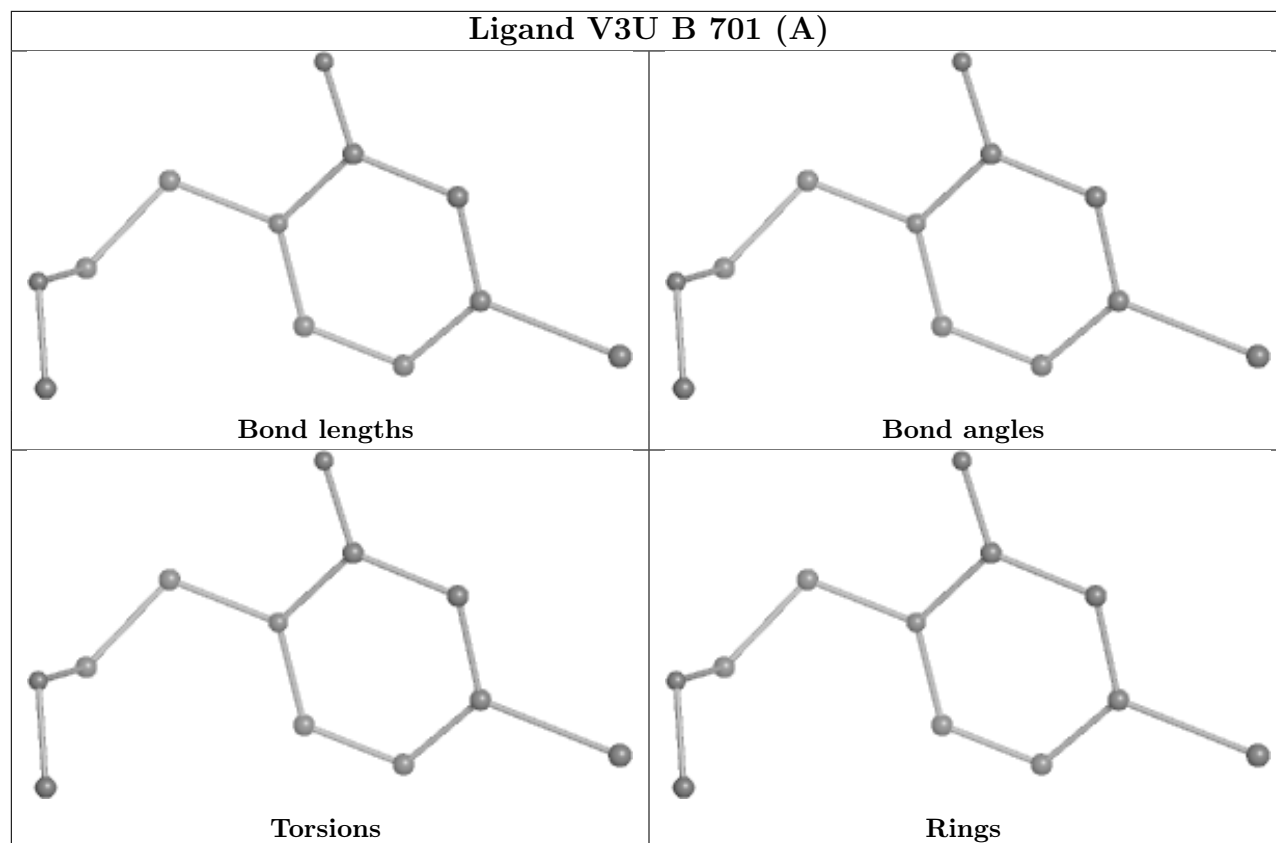


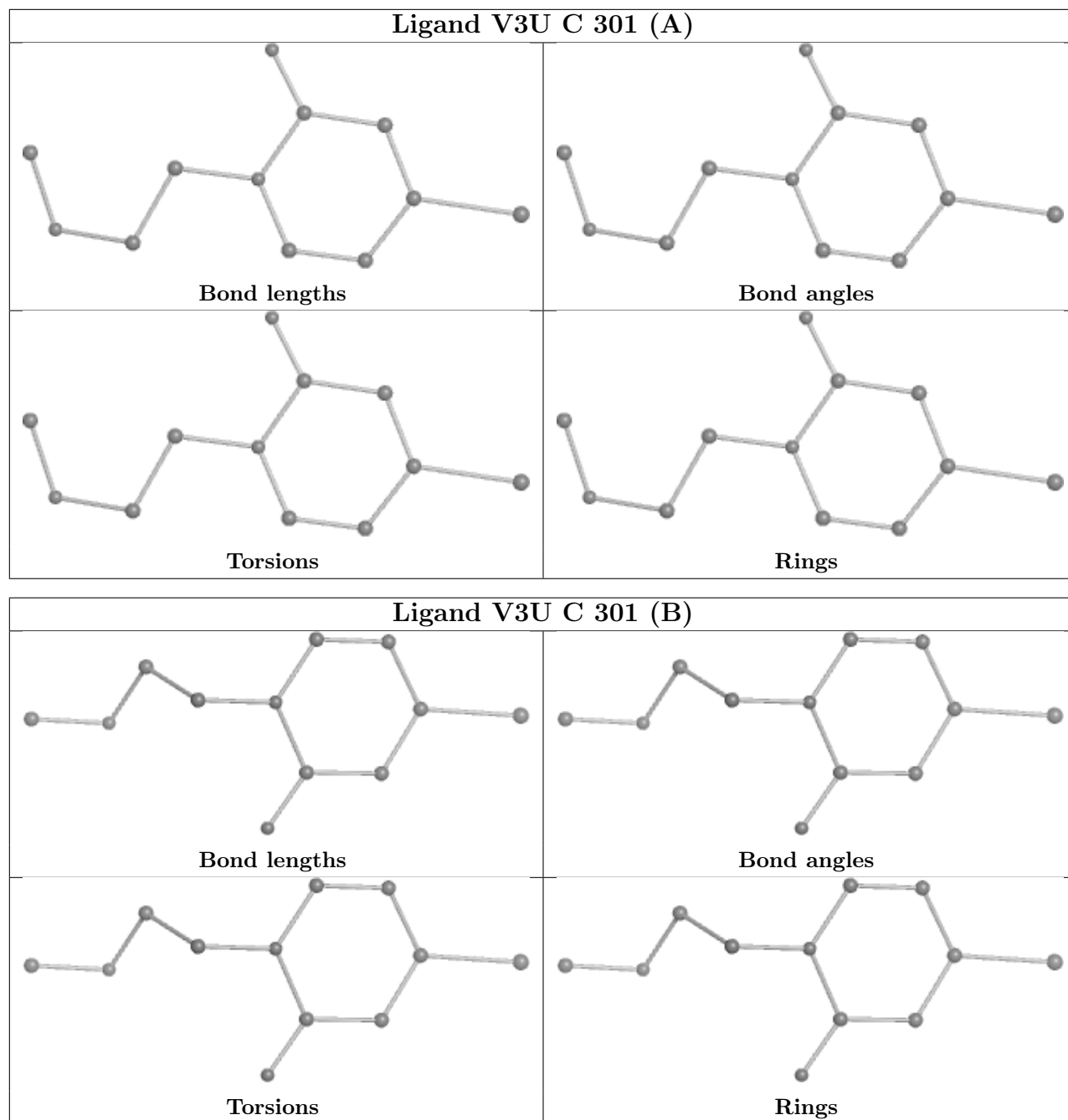
Ligand V3U A 302

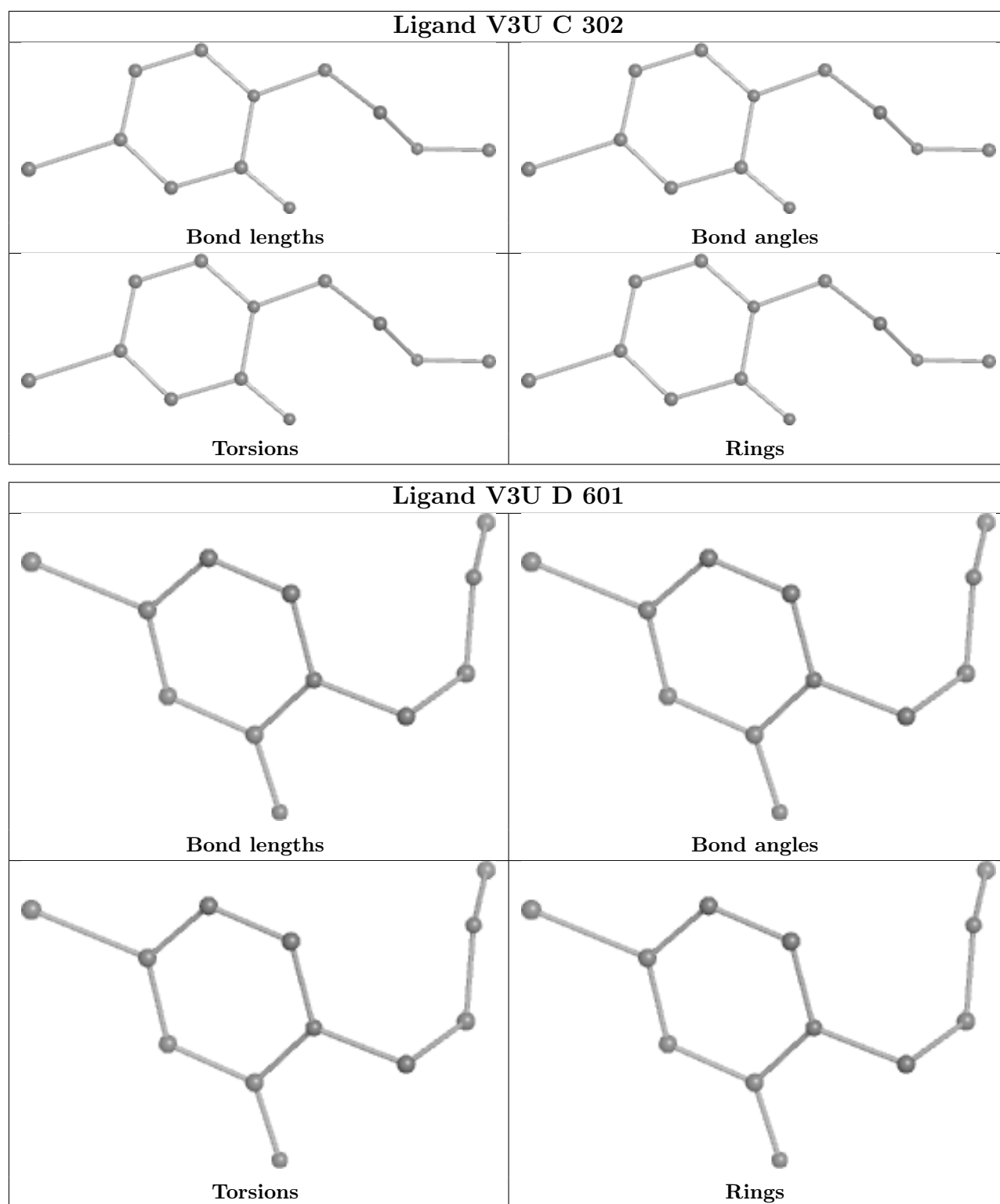


Ligand V3U A 303









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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	300/302 (99%)	0.14	19 (6%) 27 25	27, 50, 111, 143	2 (0%)
1	C	268/302 (88%)	0.55	21 (7%) 20 18	29, 66, 108, 138	1 (0%)
2	B	262/268 (97%)	-0.02	7 (2%) 56 53	24, 52, 77, 105	1 (0%)
2	D	262/268 (97%)	0.72	35 (13%) 8 7	28, 72, 120, 159	1 (0%)
All	All	1092/1140 (95%)	0.34	82 (7%) 22 20	24, 58, 112, 159	5 (0%)

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	432	VAL	7.1
1	C	296	LEU	6.5
1	C	250	LYS	4.8
1	A	15	TYR	4.1
2	B	391	LEU	4.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	A	160	11/12	0.98	0.06	41,44,49,50	0
1	TPO	C	160	11/12	0.98	0.05	48,56,63,65	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

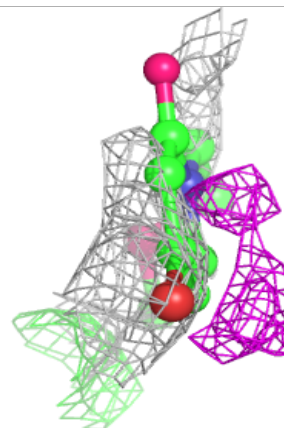
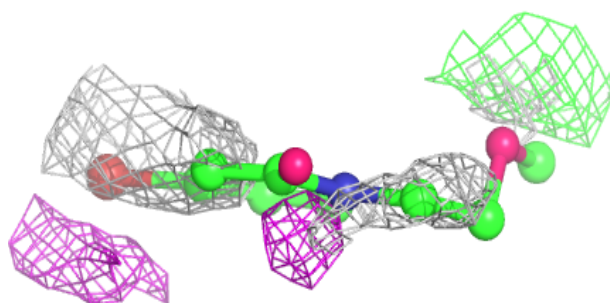
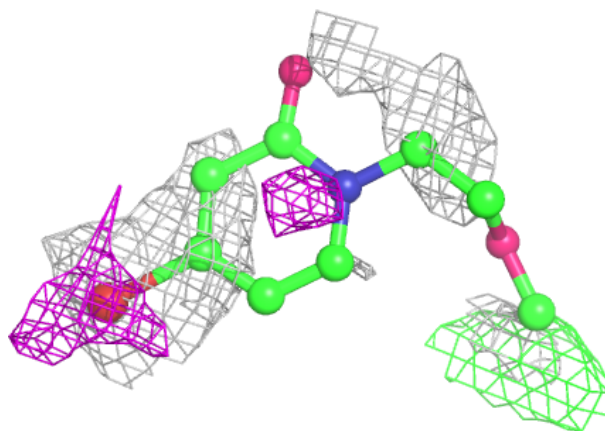
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	V3U	A	303	12/12	0.69	0.22	119,143,162,198	0
3	V3U	B	701[A]	12/12	0.71	0.55	106,112,132,137	12
3	V3U	B	701[B]	12/12	0.71	0.55	106,112,132,137	12
3	V3U	C	302	12/12	0.73	0.20	129,143,157,187	0
3	V3U	C	301[B]	12/12	0.80	0.38	95,102,109,109	12
3	V3U	C	301[A]	12/12	0.80	0.38	105,111,117,118	12
3	V3U	A	301	12/12	0.82	0.25	73,81,99,102	0
3	V3U	A	302	12/12	0.83	0.20	76,97,119,120	0
3	V3U	D	601	12/12	0.96	0.11	60,67,72,74	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.

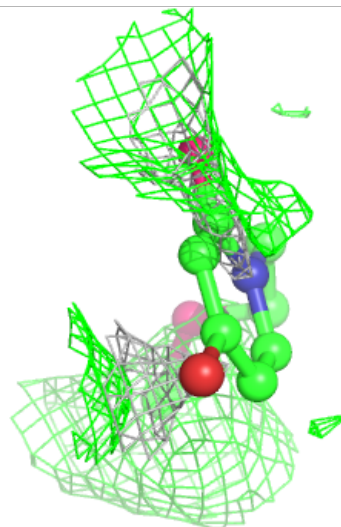
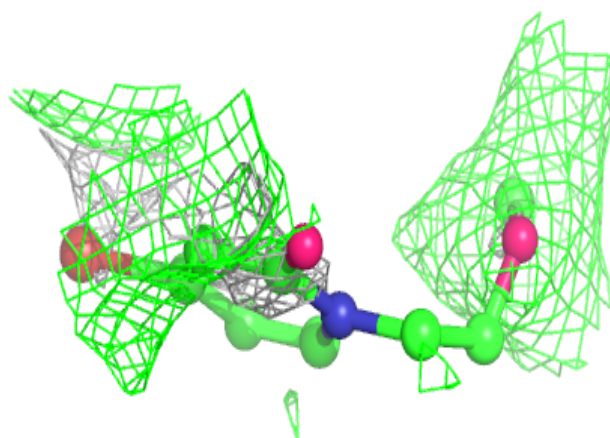
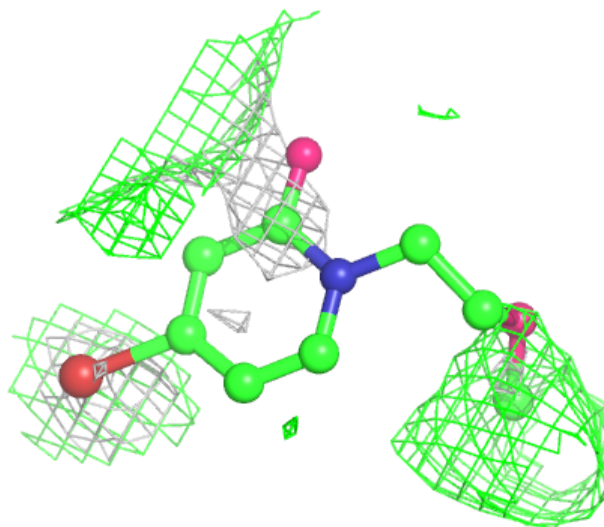
Electron density around V3U A 303:

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



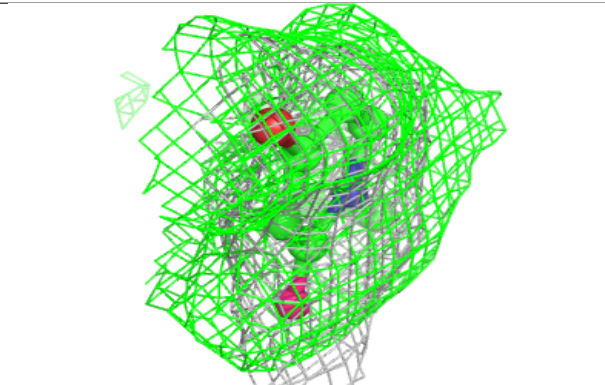
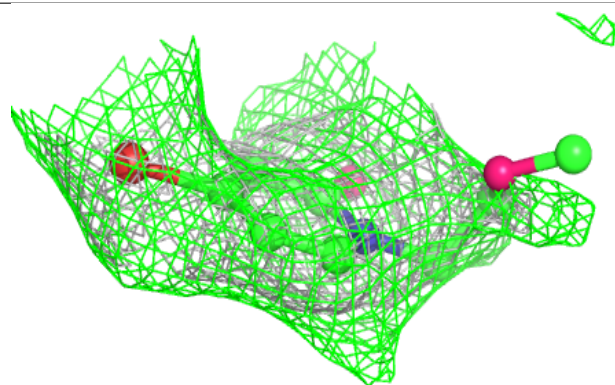
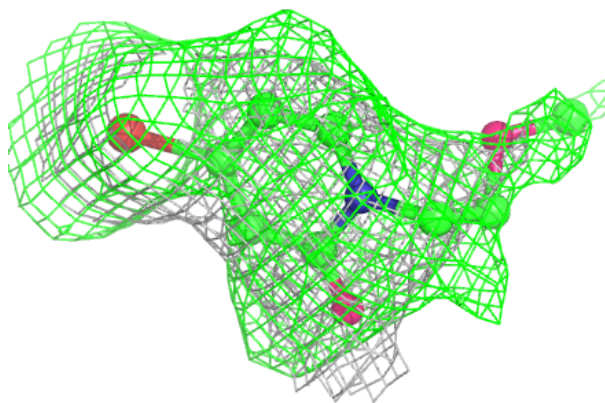
Electron density around V3U B 701 (A):

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

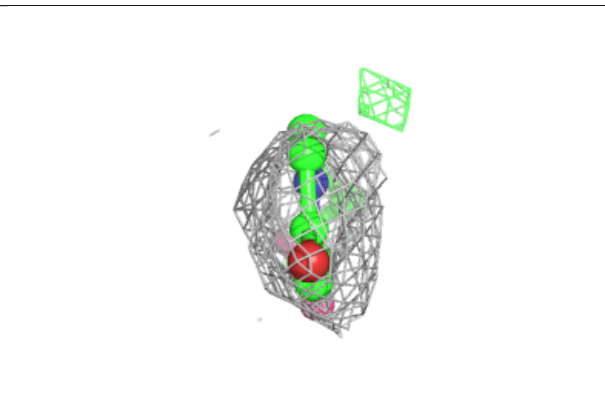
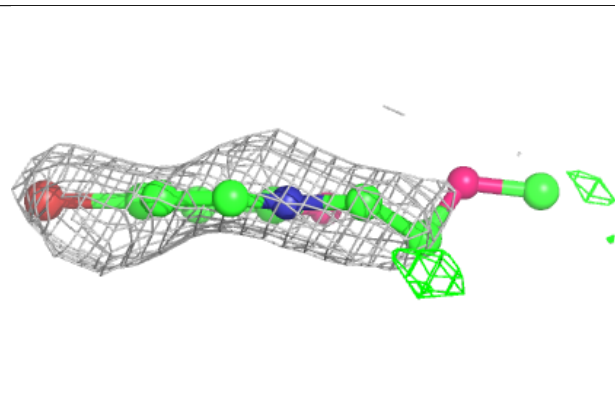
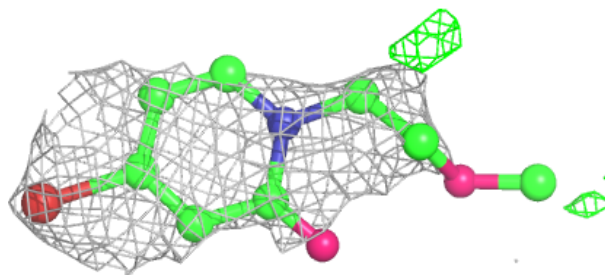


Electron density around V3U B 701 (B):

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

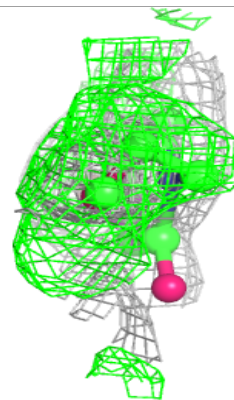
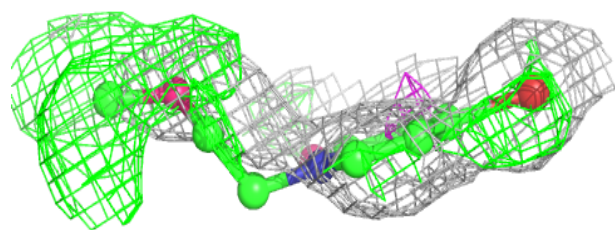
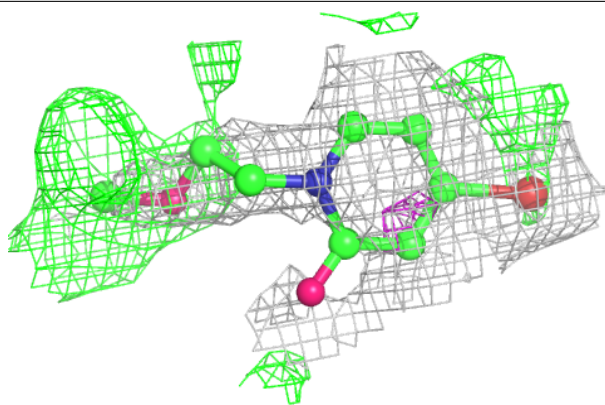
**Electron density around V3U C 302:**

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

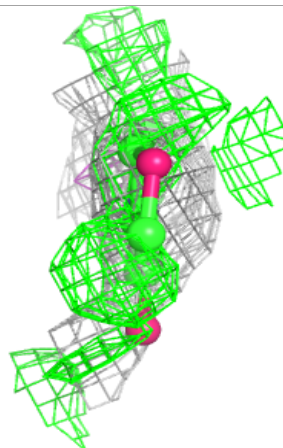
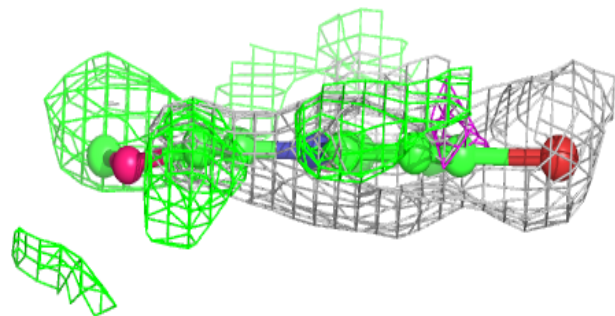
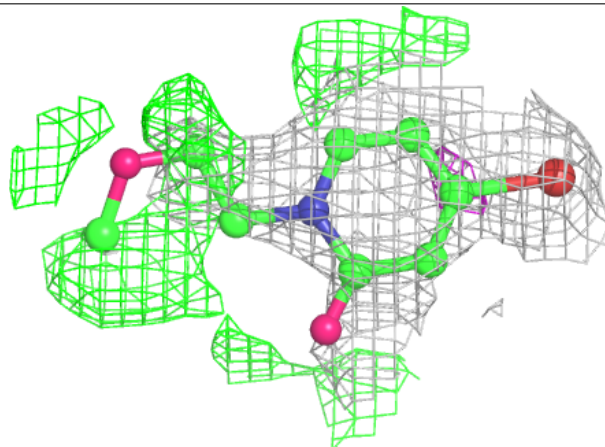


Electron density around V3U C 301 (B):

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

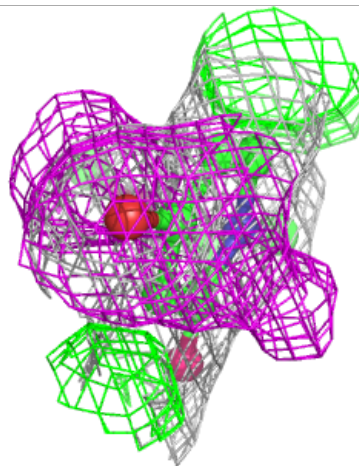
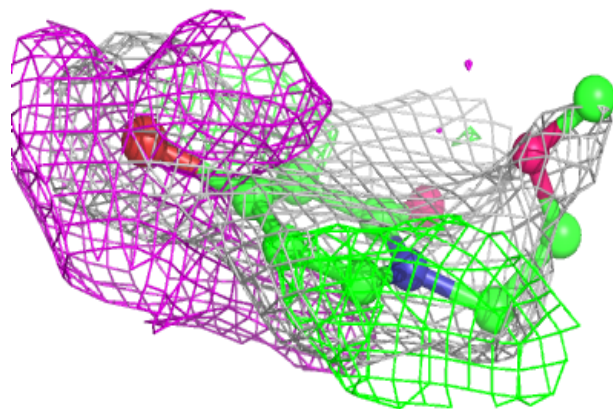
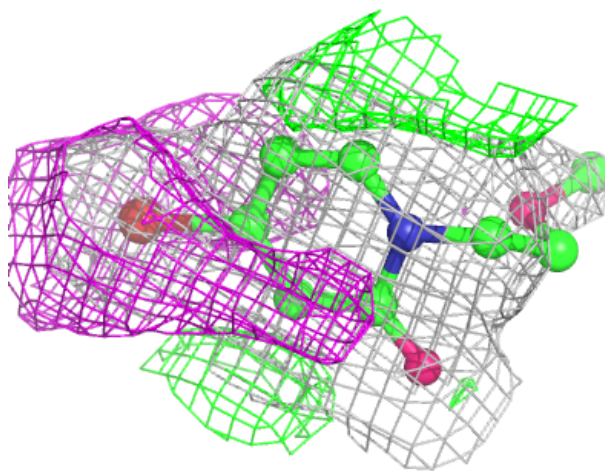
**Electron density around V3U C 301 (A):**

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



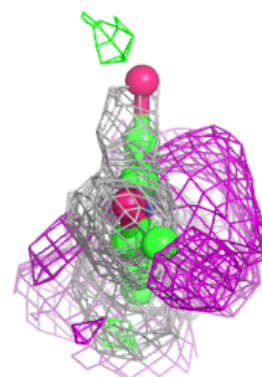
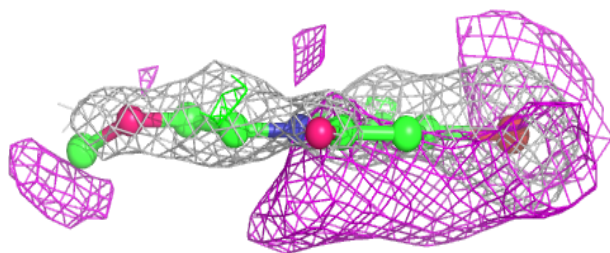
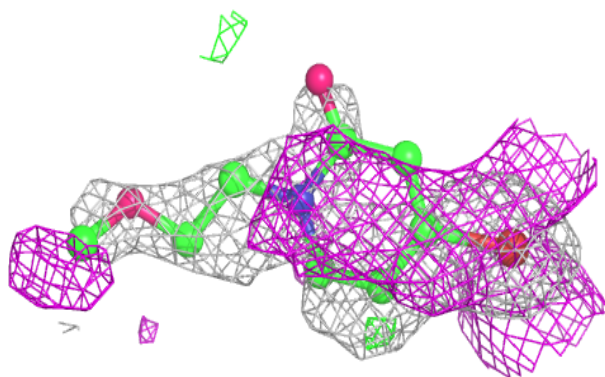
Electron density around V3U A 301:

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

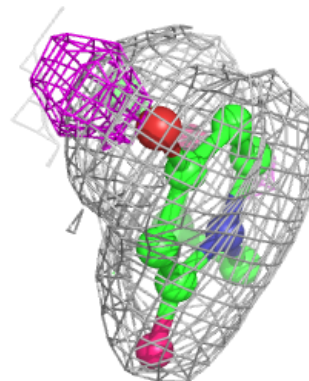
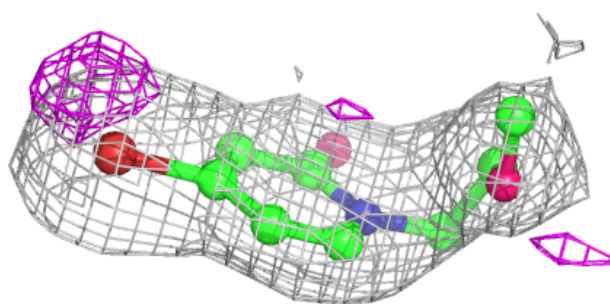
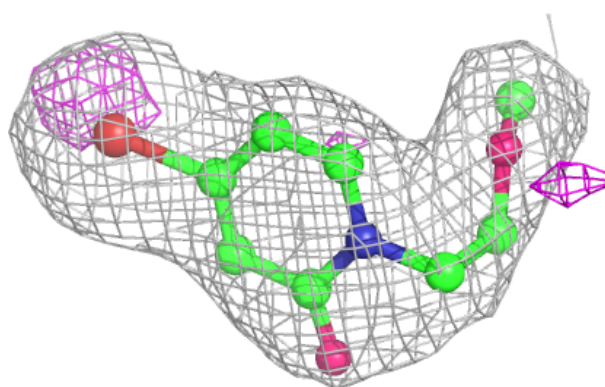


Electron density around V3U A 302:

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

**Electron density around V3U D 601:**

$2mF_o-DF_c$ (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.