



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:03 AM UTC

PDB ID : 6K0R / pdb_00006k0r
Title : Ruvbl1-Ruvbl2 with truncated domain II in complex with phosphorylated Cordycepin
Authors : Zhang, W.; Chen, L.; Li, W.; Ju, D.; Huang, N.; Zhang, E.
Deposited on : 2019-05-07
Resolution : 2.50 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

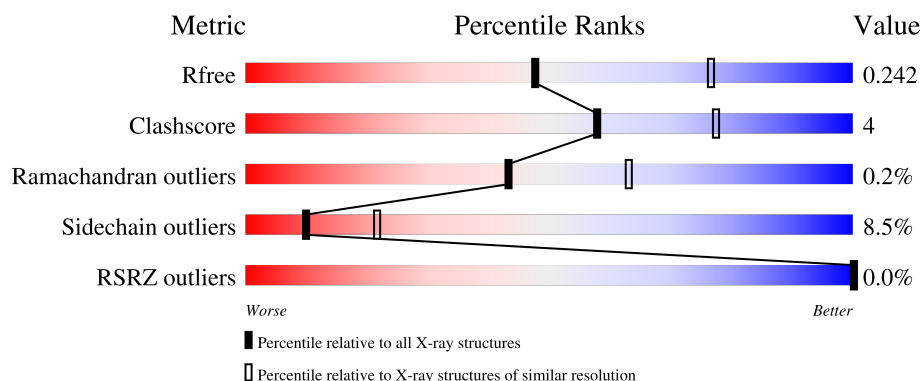
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	355	 72% 15% • 11%
1	B	355	 72% 16% • 10%
1	C	355	 70% 18% 12%
1	G	355	 78% 9% • 12%
1	H	355	 76% 13% • 10%

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Mol	Chain	Length	Quality of chain
1	I	355	
2	D	366	
2	E	366	
2	F	366	
2	J	366	
2	K	366	
2	L	366	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27180 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 RuvB-like 1, RuvB-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2286	1437	393	445	11			
1	B	318	Total	C	N	O	S	0	0	0
			2292	1445	387	449	11			
1	C	313	Total	C	N	O	S	0	0	0
			2320	1462	407	440	11			
1	G	311	Total	C	N	O	S	0	0	0
			2211	1394	382	425	10			
1	H	318	Total	C	N	O	S	0	0	0
			2338	1474	407	446	11			
1	I	313	Total	C	N	O	S	0	0	0
			2273	1431	388	443	11			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9Y265
A	0	PRO	-	expression tag	UNP Q9Y265
A	1	SER	-	expression tag	UNP Q9Y265
A	230	GLY	-	linker	UNP Q9Y265
A	231	PRO	-	linker	UNP Q9Y265
A	232	PRO	-	linker	UNP Q9Y265
A	233	GLY	-	linker	UNP Q9Y265
B	-1	GLY	-	expression tag	UNP Q9Y265
B	0	PRO	-	expression tag	UNP Q9Y265
B	1	SER	-	expression tag	UNP Q9Y265
B	230	GLY	-	linker	UNP Q9Y265
B	231	PRO	-	linker	UNP Q9Y265
B	232	PRO	-	linker	UNP Q9Y265
B	233	GLY	-	linker	UNP Q9Y265
C	-1	GLY	-	expression tag	UNP Q9Y265
C	0	PRO	-	expression tag	UNP Q9Y265
C	1	SER	-	expression tag	UNP Q9Y265

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Chain	Residue	Modelled	Actual	Comment	Reference
C	230	GLY	-	linker	UNP Q9Y265
C	231	PRO	-	linker	UNP Q9Y265
C	232	PRO	-	linker	UNP Q9Y265
C	233	GLY	-	linker	UNP Q9Y265
G	-1	GLY	-	expression tag	UNP Q9Y265
G	0	PRO	-	expression tag	UNP Q9Y265
G	1	SER	-	expression tag	UNP Q9Y265
G	230	GLY	-	linker	UNP Q9Y265
G	231	PRO	-	linker	UNP Q9Y265
G	232	PRO	-	linker	UNP Q9Y265
G	233	GLY	-	linker	UNP Q9Y265
H	-1	GLY	-	expression tag	UNP Q9Y265
H	0	PRO	-	expression tag	UNP Q9Y265
H	1	SER	-	expression tag	UNP Q9Y265
H	230	GLY	-	linker	UNP Q9Y265
H	231	PRO	-	linker	UNP Q9Y265
H	232	PRO	-	linker	UNP Q9Y265
H	233	GLY	-	linker	UNP Q9Y265
I	-1	GLY	-	expression tag	UNP Q9Y265
I	0	PRO	-	expression tag	UNP Q9Y265
I	1	SER	-	expression tag	UNP Q9Y265
I	230	GLY	-	linker	UNP Q9Y265
I	231	PRO	-	linker	UNP Q9Y265
I	232	PRO	-	linker	UNP Q9Y265
I	233	GLY	-	linker	UNP Q9Y265

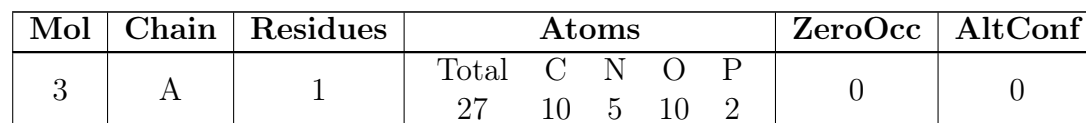
- Molecule 2 is a protein called RuvB-like 2,RuvB-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	303	Total	C	N	O	S	0	0	0
			2197	1382	379	425	11			
2	E	304	Total	C	N	O	S	0	0	0
			2224	1395	388	430	11			
2	F	307	Total	C	N	O	S	0	0	0
			2278	1429	404	433	12			
2	J	302	Total	C	N	O	S	0	0	0
			2151	1347	382	410	12			
2	K	300	Total	C	N	O	S	0	0	0
			2161	1352	379	418	12			
2	L	300	Total	C	N	O	S	0	0	0
			2129	1338	372	409	10			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP Q9Y230
D	-1	GLY	-	expression tag	UNP Q9Y230
D	0	SER	-	expression tag	UNP Q9Y230
D	234	GLY	-	linker	UNP Q9Y230
D	235	PRO	-	linker	UNP Q9Y230
D	236	PRO	-	linker	UNP Q9Y230
D	237	GLY	-	linker	UNP Q9Y230
E	-2	GLY	-	expression tag	UNP Q9Y230
E	-1	GLY	-	expression tag	UNP Q9Y230
E	0	SER	-	expression tag	UNP Q9Y230
E	234	GLY	-	linker	UNP Q9Y230
E	235	PRO	-	linker	UNP Q9Y230
E	236	PRO	-	linker	UNP Q9Y230
E	237	GLY	-	linker	UNP Q9Y230
F	-2	GLY	-	expression tag	UNP Q9Y230
F	-1	GLY	-	expression tag	UNP Q9Y230
F	0	SER	-	expression tag	UNP Q9Y230
F	234	GLY	-	linker	UNP Q9Y230
F	235	PRO	-	linker	UNP Q9Y230
F	236	PRO	-	linker	UNP Q9Y230
F	237	GLY	-	linker	UNP Q9Y230
J	-2	GLY	-	expression tag	UNP Q9Y230
J	-1	GLY	-	expression tag	UNP Q9Y230
J	0	SER	-	expression tag	UNP Q9Y230
J	234	GLY	-	linker	UNP Q9Y230
J	235	PRO	-	linker	UNP Q9Y230
J	236	PRO	-	linker	UNP Q9Y230
J	237	GLY	-	linker	UNP Q9Y230
K	-2	GLY	-	expression tag	UNP Q9Y230
K	-1	GLY	-	expression tag	UNP Q9Y230
K	0	SER	-	expression tag	UNP Q9Y230
K	234	GLY	-	linker	UNP Q9Y230
K	235	PRO	-	linker	UNP Q9Y230
K	236	PRO	-	linker	UNP Q9Y230
K	237	GLY	-	linker	UNP Q9Y230
L	-2	GLY	-	expression tag	UNP Q9Y230
L	-1	GLY	-	expression tag	UNP Q9Y230
L	0	SER	-	expression tag	UNP Q9Y230
L	234	GLY	-	linker	UNP Q9Y230
L	235	PRO	-	linker	UNP Q9Y230
L	236	PRO	-	linker	UNP Q9Y230
L	237	GLY	-	linker	UNP Q9Y230

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 26	C 10	N 5	O 9	P 2	0	0
4	C	1	Total 26	C 10	N 5	O 9	P 2	0	0

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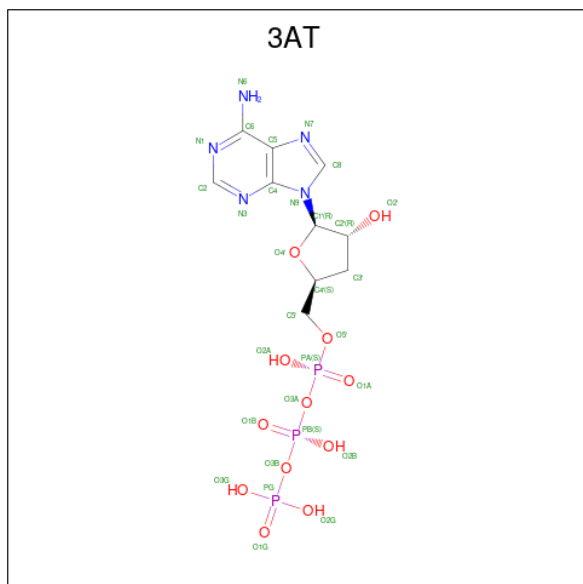
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	F	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	G	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	H	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	I	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	K	1	Total	C	N	O	P	0	0
			26	10	5	9	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

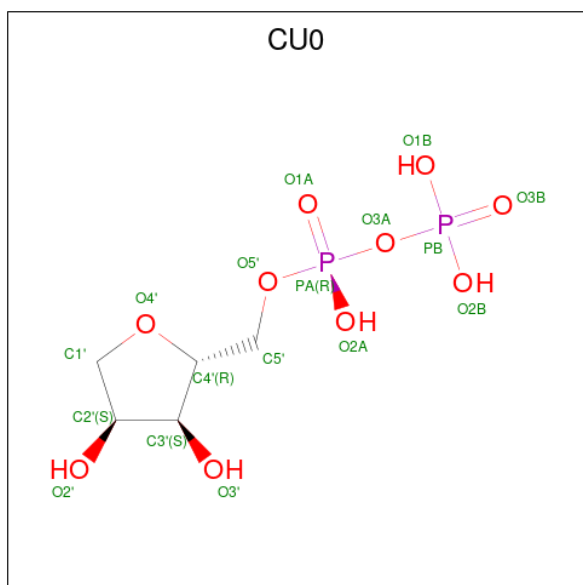
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Mg	0	0
			1	1		
5	L	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (CCD ID: 3AT) (formula: C₁₀H₁₆N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	J	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 7 is [(2 {R},3 {S},4 {S})-3,4-bis(oxidanyl)oxolan-2-yl]methyl phosphono hydrogen phosphate (CCD ID: CU0) (formula: C₅H₁₂O₁₀P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	O	P	0	0
			17	5	10	2		

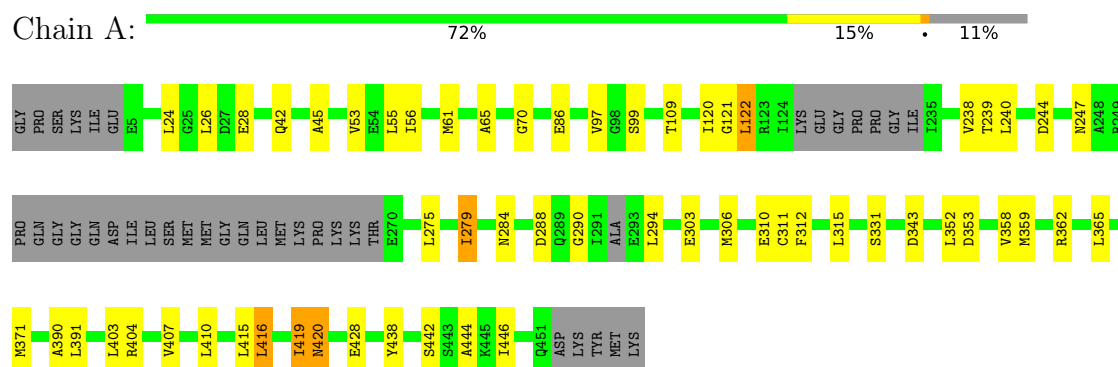
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			1	1		
8	E	2	Total	O	0	0
			2	2		
8	F	2	Total	O	0	0
			2	2		
8	J	1	Total	O	0	0
			1	1		

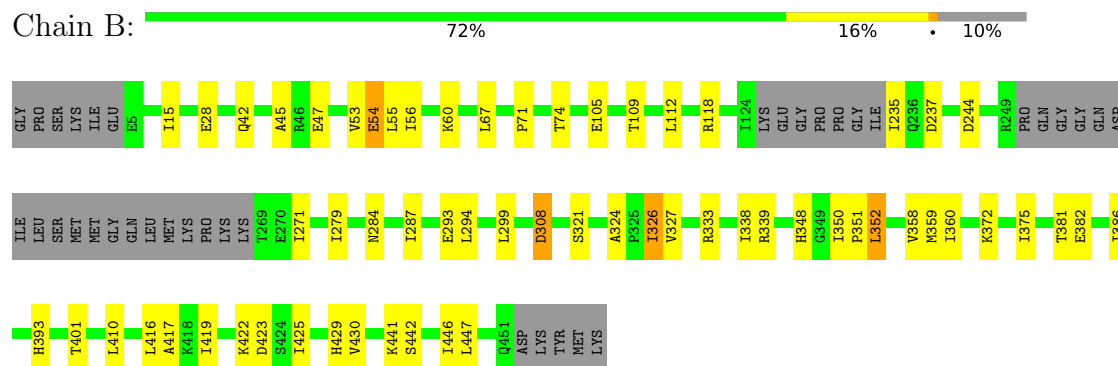
3 Residue-property plots

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.

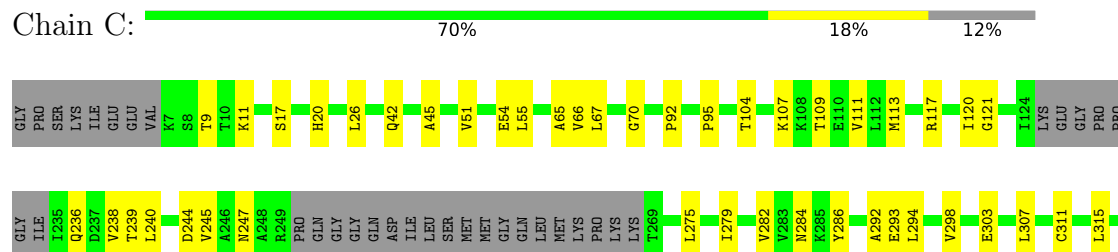
- Molecule 1: RuvB-like 1,RuvB-like 1



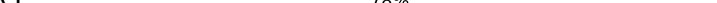
- Molecule 1: RuvB-like 1,RuvB-like 1

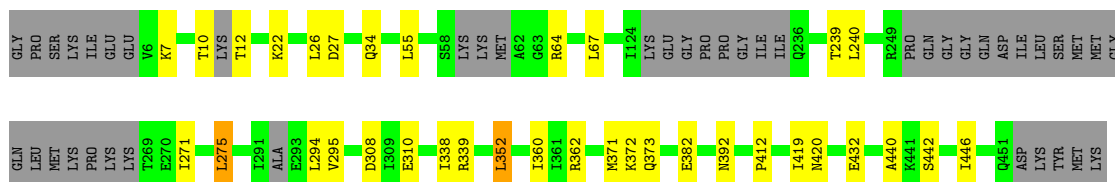


- Molecule 1: RuvB-like 1,RuvB-like 1

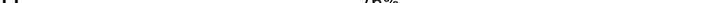


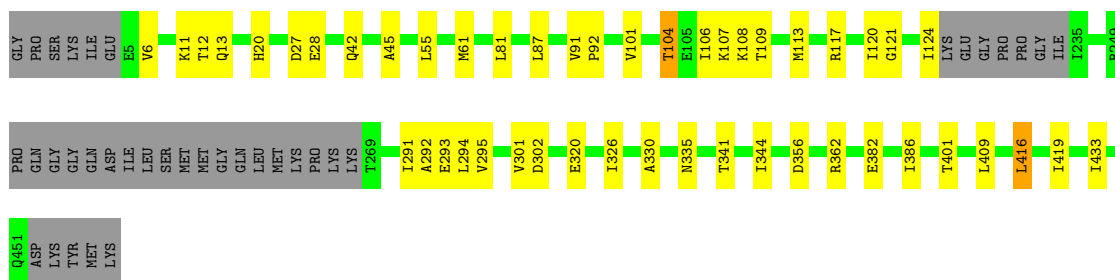
- Molecule 1: RuvB-like 1, RuvB-like 1

Chain G:  78% 9% • 12%



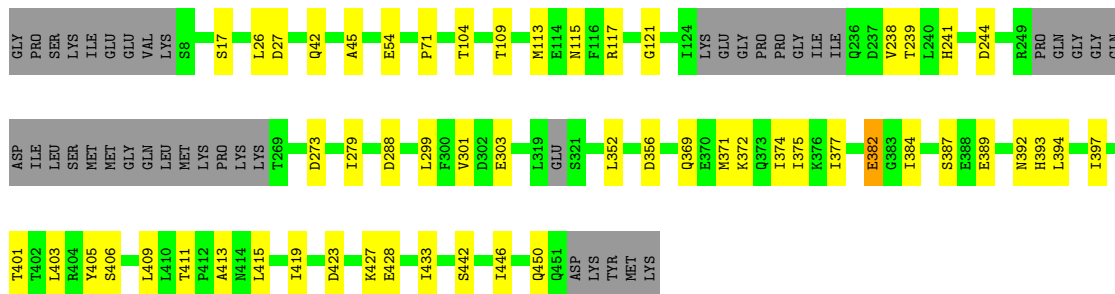
- Molecule 1: RuvB-like 1, RuvB-like 1

Chain H:  76% 13% 10%

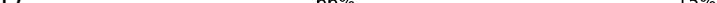


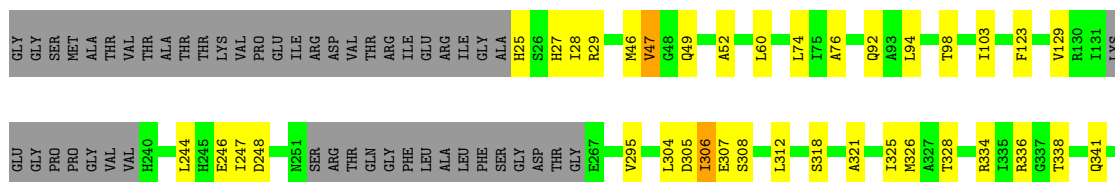
- Molecule 1: RuvB-like 1, RuvB-like 1

Chain I: 73% 15% 12%



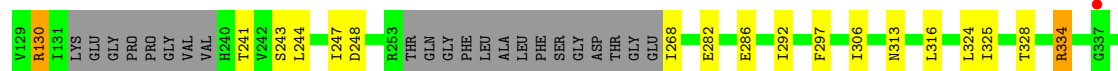
- Molecule 2: RuvB-like 2, RuvB-like 2

Chain D:  66% 15% • 17%

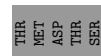
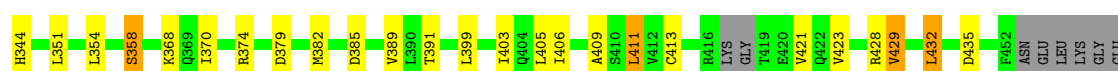
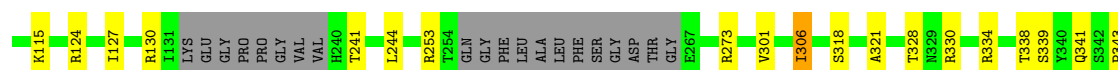




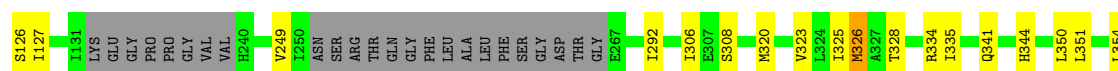
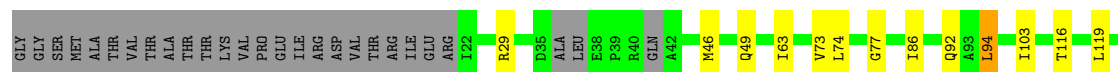
- Molecule 2: RuvB-like 2,RuvB-like 2



- Molecule 2: RuvB-like 2,RuvB-like 2



- Molecule 2: RuvB-like 2,RuvB-like 2



- Molecule 2: RuvB-like 2,RuvB-like 2

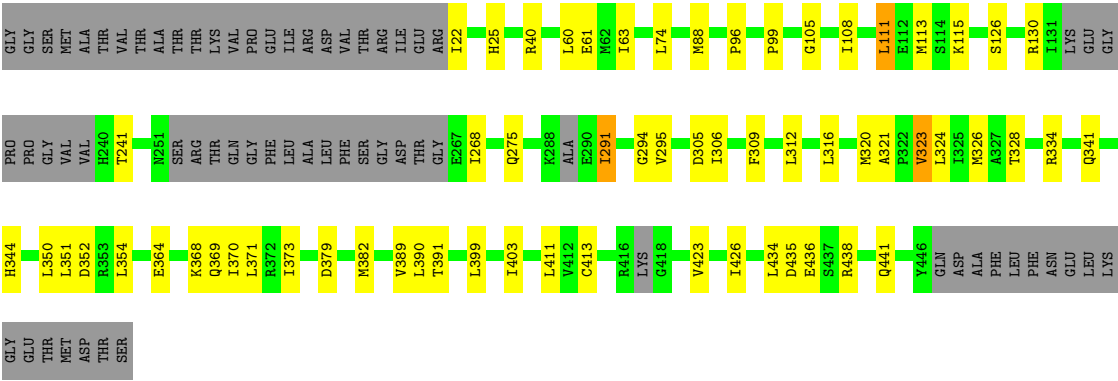
Chain K:

65%

16%

•

18%



• Molecule 2: RuvB-like 2,RuvB-like 2

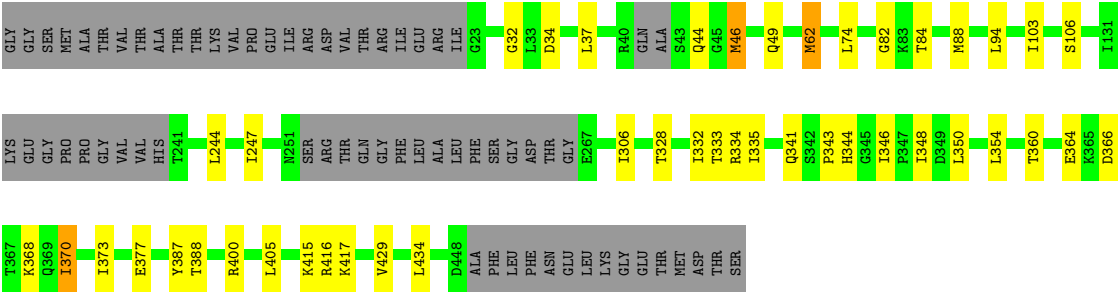
Chain L:

70%

11%

•

18%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.30Å 186.42Å 235.18Å 90.00° 91.04° 90.00°	Depositor
Resolution (Å)	49.72 – 2.50 49.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	55.7 (49.72-2.50) 55.7 (49.72-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.228 , 0.269 0.240 , 0.242	Depositor DCC
R_{free} test set	4736 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.044 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.044 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.044 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.038 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.219 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27180	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: CUU, MG, ADP, 3AT, CU0

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	0.78	0/2312	1.42	3/3143 (0.1%)
1	B	0.80	1/2318 (0.0%)	1.40	4/3151 (0.1%)
1	C	0.78	0/2345	1.40	8/3172 (0.3%)
1	G	0.80	0/2234	1.41	0/3039
1	H	0.81	0/2365	1.42	5/3208 (0.2%)
1	I	0.80	1/2298 (0.0%)	1.39	2/3119 (0.1%)
2	D	0.81	1/2224 (0.0%)	1.38	1/3023 (0.0%)
2	E	0.79	0/2249	1.42	7/3050 (0.2%)
2	F	0.77	0/2304	1.38	1/3118 (0.0%)
2	J	0.80	0/2174	1.43	11/2947 (0.4%)
2	K	0.79	0/2182	1.43	11/2959 (0.4%)
2	L	0.79	0/2154	1.37	3/2927 (0.1%)
All	All	0.79	3/27159 (0.0%)	1.40	56/36856 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	401	THR	CA-C	6.36	1.55	1.52
2	D	397	THR	CA-C	6.16	1.55	1.52
1	I	401	THR	CA-C	5.96	1.55	1.52

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	417	LYS	CA-C-N	6.53	126.31	120.10
2	J	417	LYS	C-N-CA	6.53	126.31	120.10
2	K	111	LEU	CA-C-N	6.22	129.76	120.31
2	K	111	LEU	C-N-CA	6.22	129.76	120.31
2	L	49	GLN	CA-C-N	6.04	128.29	120.44

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	2286	0	2226	23	0
1	B	2292	0	2245	22	0
1	C	2320	0	2342	28	0
1	G	2211	0	2137	10	0
1	H	2338	0	2339	16	0
1	I	2273	0	2244	20	0
2	D	2197	0	2111	26	0
2	E	2224	0	2159	26	0
2	F	2278	0	2233	31	0
2	J	2151	0	2045	20	0
2	K	2161	0	2095	24	0
2	L	2129	0	2013	20	0
3	A	27	0	12	0	0
4	B	26	0	0	0	0
4	C	26	0	0	0	0
4	D	26	0	0	0	0
4	F	26	0	0	3	0
4	G	26	0	0	0	0
4	H	26	0	0	0	0
4	I	26	0	0	0	0
4	K	26	0	0	1	0
5	D	1	0	0	0	0
5	L	1	0	0	0	0
6	E	30	0	12	0	0
6	J	30	0	12	0	0
7	L	17	0	0	2	0
8	A	1	0	0	0	0
8	E	2	0	0	0	0
8	F	2	0	0	0	0
8	J	1	0	0	0	0
All	All	27180	0	26225	240	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 4.

The worst 5 of 240 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)
2:D:382:MET:HB3	2:D:421:VAL:HB	1.59	0.85
2:D:94:LEU:HD23	2:D:98:THR:HG21	1.61	0.83
1:G:362:ARG:HB2	2:K:434:LEU:HD11	1.65	0.79
1:C:9:THR:HG21	1:C:245:VAL:HG21	1.68	0.75
2:L:84:THR:HB	7:L:501:CU0:O1A	1.88	0.73

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	308/355 (87%)	288 (94%)	19 (6%)	1 (0%)	36	55
1	B	312/355 (88%)	301 (96%)	10 (3%)	1 (0%)	36	55
1	C	303/355 (85%)	289 (95%)	13 (4%)	1 (0%)	36	55
1	G	299/355 (84%)	283 (95%)	14 (5%)	2 (1%)	18	34
1	H	312/355 (88%)	291 (93%)	20 (6%)	1 (0%)	36	55
1	I	305/355 (86%)	295 (97%)	10 (3%)	0	100	100
2	D	297/366 (81%)	288 (97%)	9 (3%)	0	100	100
2	E	296/366 (81%)	286 (97%)	10 (3%)	0	100	100
2	F	297/366 (81%)	293 (99%)	4 (1%)	0	100	100
2	J	290/366 (79%)	278 (96%)	10 (3%)	2 (1%)	18	34
2	K	290/366 (79%)	279 (96%)	11 (4%)	0	100	100
2	L	292/366 (80%)	280 (96%)	11 (4%)	1 (0%)	36	55
All	All	3601/4326 (83%)	3451 (96%)	141 (4%)	9 (0%)	43	63

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	401	THR
2	J	416	ARG
1	B	352	LEU
1	G	352	LEU
2	L	37	LEU

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	233/299 (78%)	211 (91%)	22 (9%)	8	18
1	B	234/299 (78%)	209 (89%)	25 (11%)	6	13
1	C	243/299 (81%)	229 (94%)	14 (6%)	18	38
1	G	219/299 (73%)	200 (91%)	19 (9%)	9	21
1	H	243/299 (81%)	223 (92%)	20 (8%)	10	23
1	I	235/299 (79%)	215 (92%)	20 (8%)	10	22
2	D	215/304 (71%)	195 (91%)	20 (9%)	8	18
2	E	221/304 (73%)	203 (92%)	18 (8%)	11	23
2	F	228/304 (75%)	208 (91%)	20 (9%)	9	20
2	J	203/304 (67%)	187 (92%)	16 (8%)	11	24
2	K	214/304 (70%)	196 (92%)	18 (8%)	10	22
2	L	200/304 (66%)	183 (92%)	17 (8%)	10	22
All	All	2688/3618 (74%)	2459 (92%)	229 (8%)	10	22

5 of 229 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	413	CYS
2	L	335	ILE
1	H	87	LEU
2	L	332	ILE
2	K	268	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	341	GLN
2	K	25	HIS
1	G	420	ASN
2	J	422	GLN
2	L	302	HIS

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](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	CUU	I	501	-	26,28,28	2.41	10 (38%)	37,43,43	3.06	16 (43%)
4	CUU	F	501	-	26,28,28	2.48	10 (38%)	37,43,43	3.02	18 (48%)
4	CUU	B	501	-	26,28,28	2.46	10 (38%)	37,43,43	2.98	15 (40%)
4	CUU	D	501	5	26,28,28	2.50	10 (38%)	37,43,43	2.82	15 (40%)
6	3AT	E	501	-	30,32,32	2.48	15 (50%)	42,50,50	2.86	17 (40%)
6	3AT	J	501	-	30,32,32	2.77	13 (43%)	42,50,50	2.76	16 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	CU0	L	501	5	16,17,17	0.56	0	22,26,26	0.67	1 (4%)
4	CUU	H	501	-	26,28,28	2.49	10 (38%)	37,43,43	2.95	17 (45%)
4	CUU	C	501	-	26,28,28	2.46	10 (38%)	37,43,43	2.95	16 (43%)
3	ADP	A	501	-	28,29,29	0.71	1 (3%)	43,45,45	0.74	1 (2%)
4	CUU	K	501	-	26,28,28	2.51	11 (42%)	37,43,43	2.98	16 (43%)
4	CUU	G	501	-	26,28,28	2.47	10 (38%)	37,43,43	3.04	18 (48%)

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
4	CUU	I	501	-	-	8/16/28/28	0/3/3/3
4	CUU	F	501	-	-	6/16/28/28	0/3/3/3
4	CUU	B	501	-	-	4/16/28/28	0/3/3/3
4	CUU	D	501	5	-	7/16/28/28	0/3/3/3
6	3AT	E	501	-	-	7/22/34/34	0/3/3/3
6	3AT	J	501	-	-	9/22/34/34	0/3/3/3
7	CU0	L	501	5	-	8/12/25/25	0/1/1/1
4	CUU	H	501	-	-	5/16/28/28	0/3/3/3
4	CUU	C	501	-	-	4/16/28/28	0/3/3/3
3	ADP	A	501	-	-	3/16/32/32	0/3/3/3
4	CUU	K	501	-	-	7/16/28/28	0/3/3/3
4	CUU	G	501	-	-	5/16/28/28	0/3/3/3

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	501	3AT	PB-O3B	6.79	1.66	1.59
4	G	501	CUU	C8-N9	-6.64	1.26	1.37
4	K	501	CUU	C8-N9	-6.57	1.26	1.37
4	C	501	CUU	C8-N9	-6.57	1.26	1.37
4	I	501	CUU	C8-N9	-6.53	1.26	1.37

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	501	CUU	C4-N9-C8	10.05	116.29	105.74
4	G	501	CUU	C4-N9-C8	9.95	116.18	105.74
4	K	501	CUU	C4-N9-C8	9.89	116.12	105.74
4	B	501	CUU	C4-N9-C8	9.63	115.85	105.74
4	C	501	CUU	C4-N9-C8	9.40	115.61	105.74

There are no chirality outliers.

5 of 73 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ADP	C5'-O5'-PA-O1A
3	A	501	ADP	C5'-O5'-PA-O2A
3	A	501	ADP	C5'-O5'-PA-O3A
4	B	501	CUU	C5'-O5'-PA-O2A
4	B	501	CUU	C5'-O5'-PA-O1A

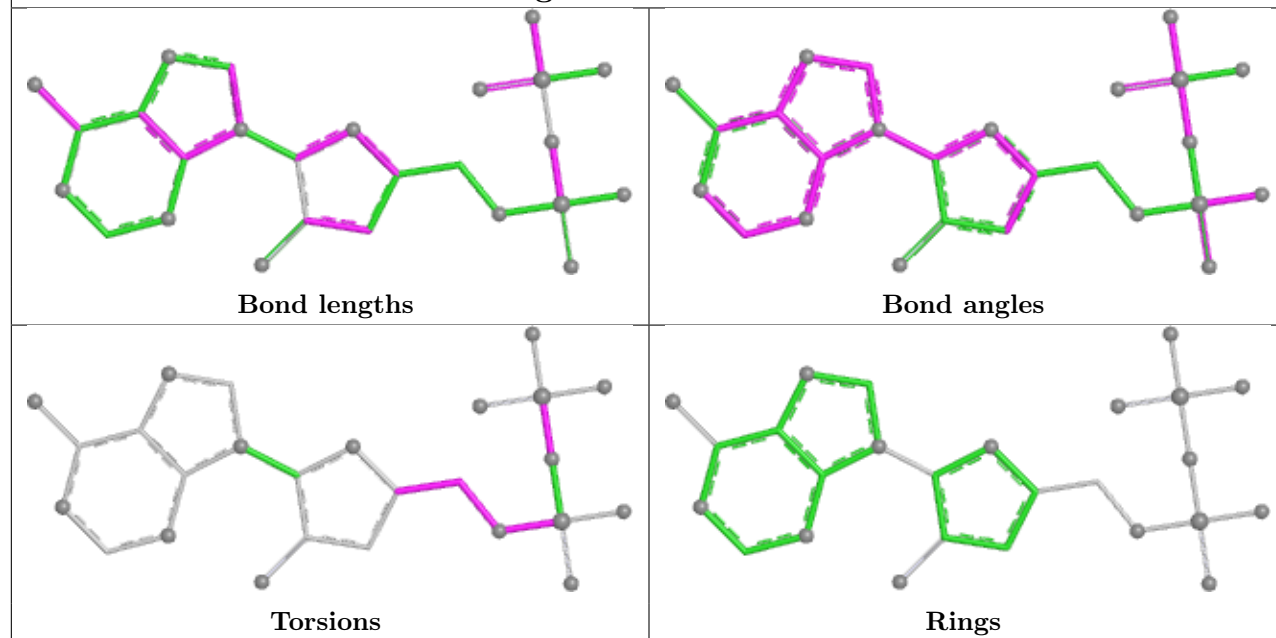
There are no ring outliers.

3 monomers are involved in 6 short contacts:

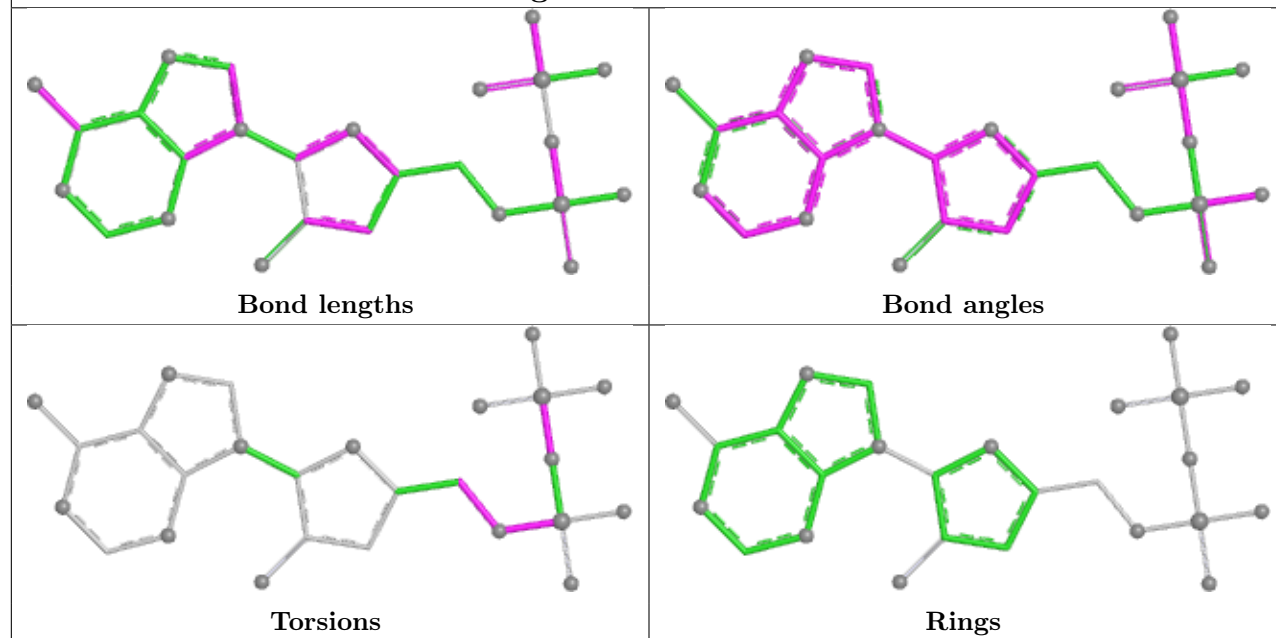
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	501	CUU	3	0
7	L	501	CU0	2	0
4	K	501	CUU	1	0

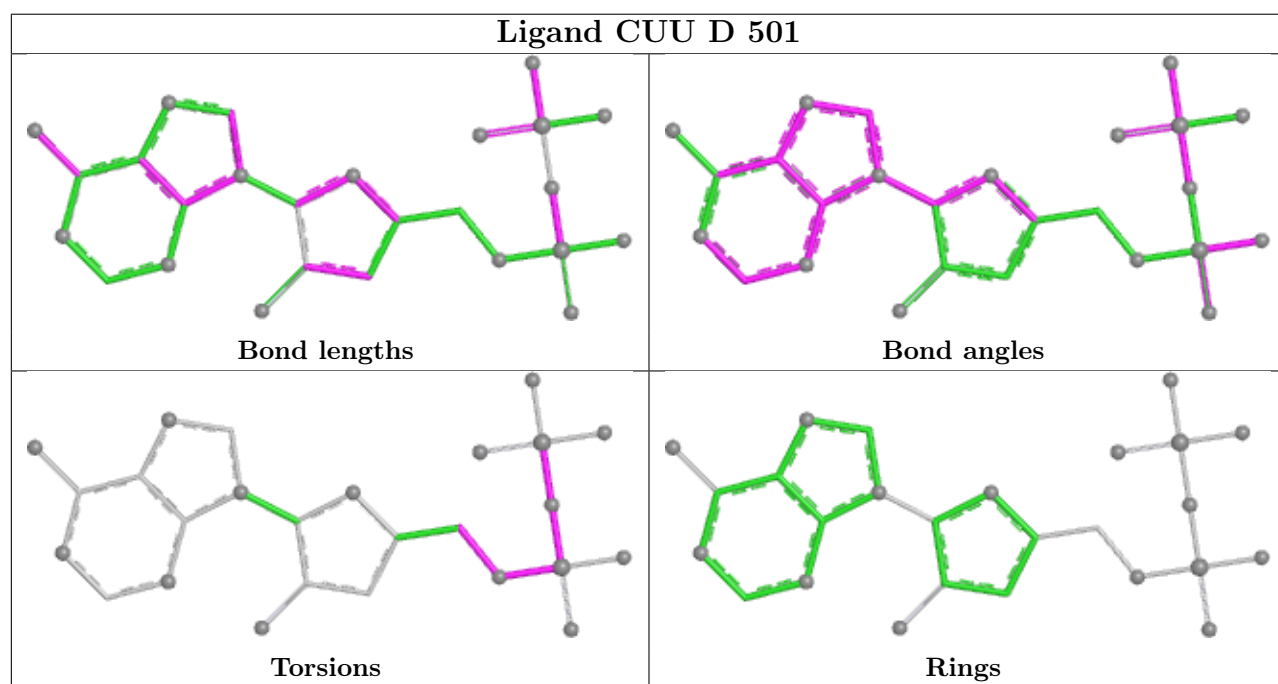
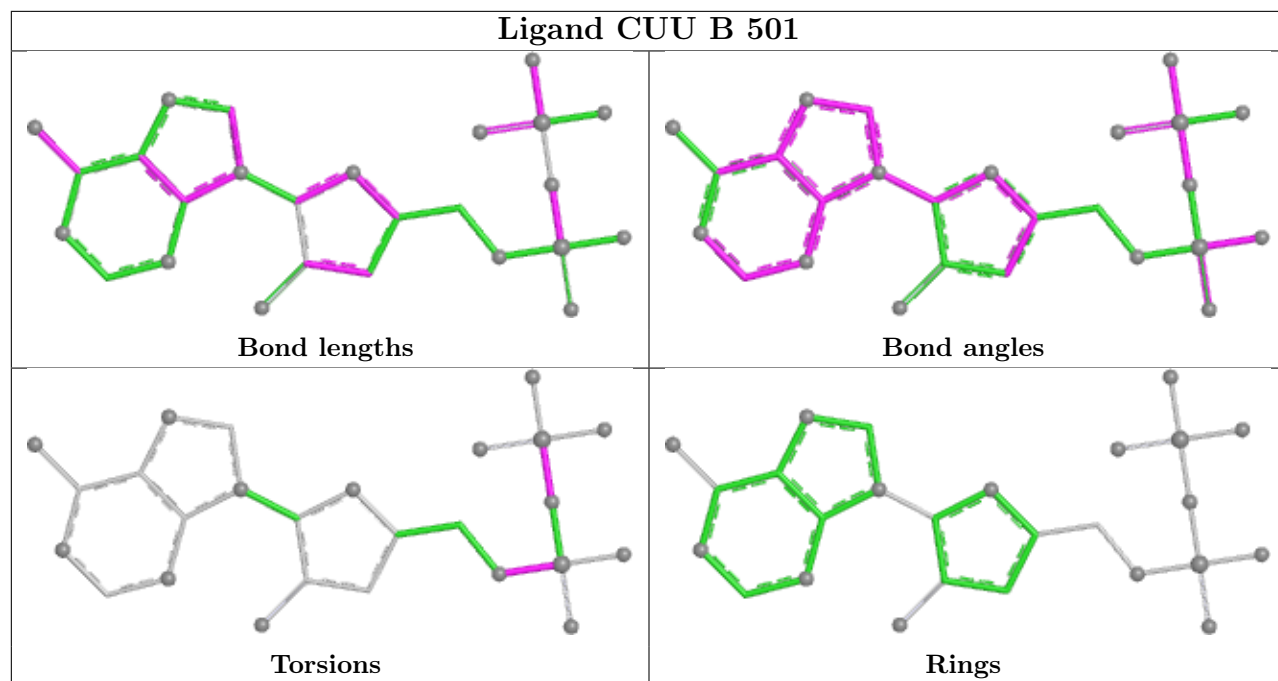
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 CUU I 501

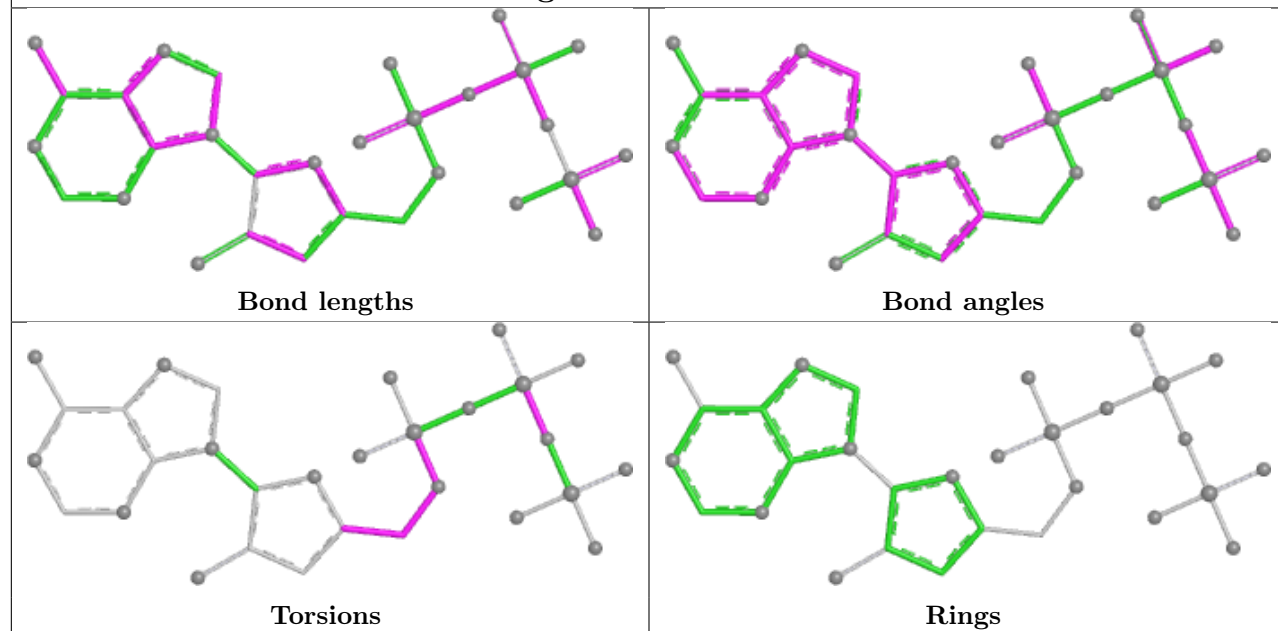


Ligand CUU F 501

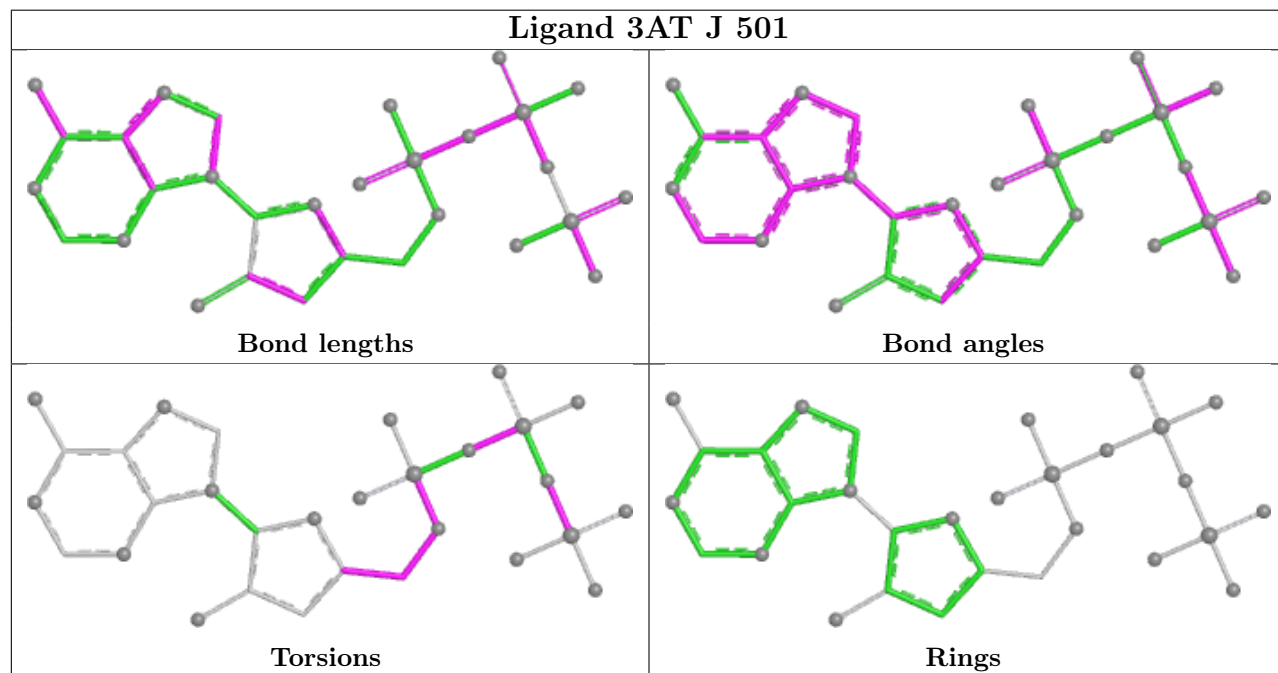




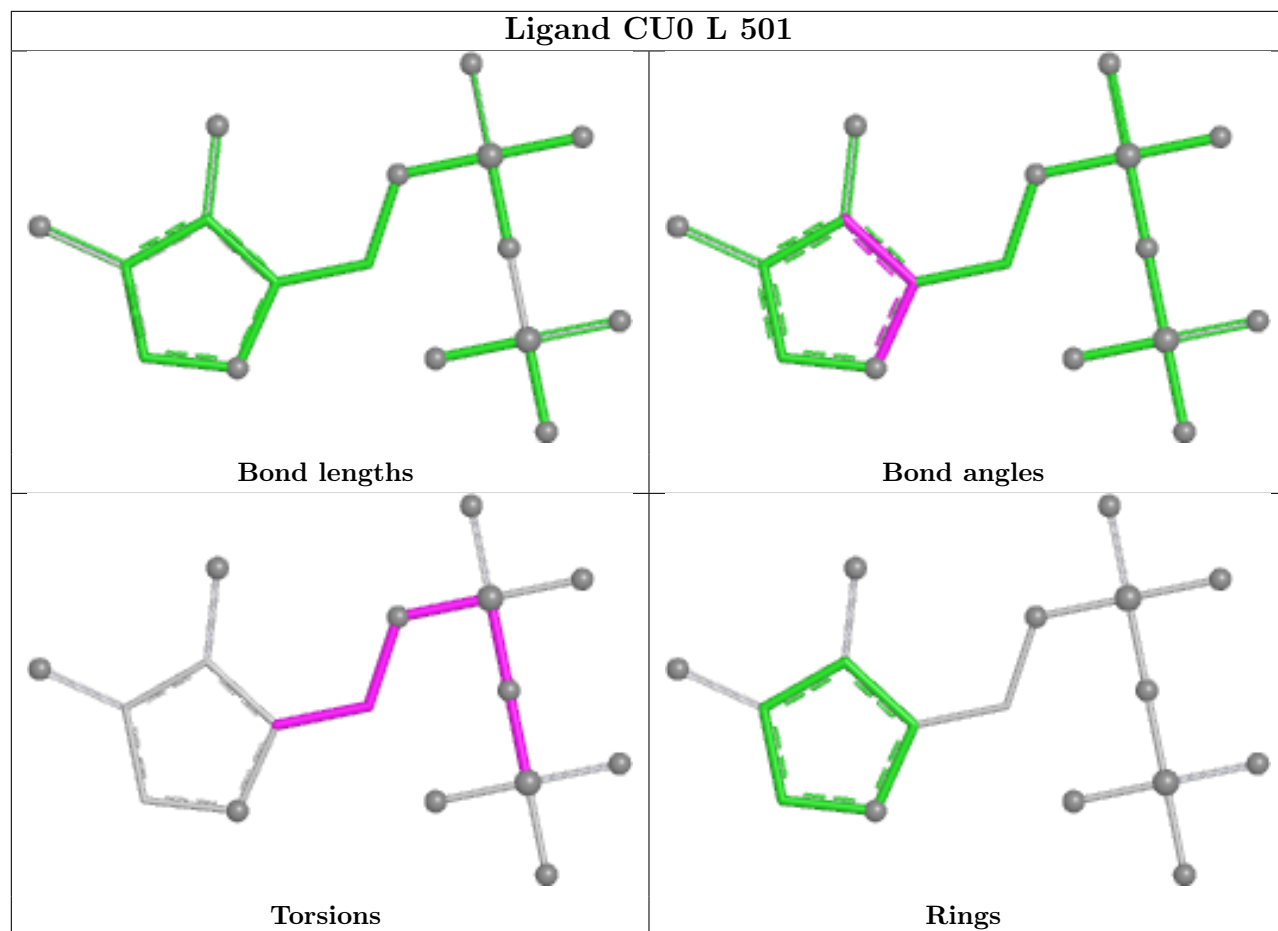
Ligand 3AT E 501



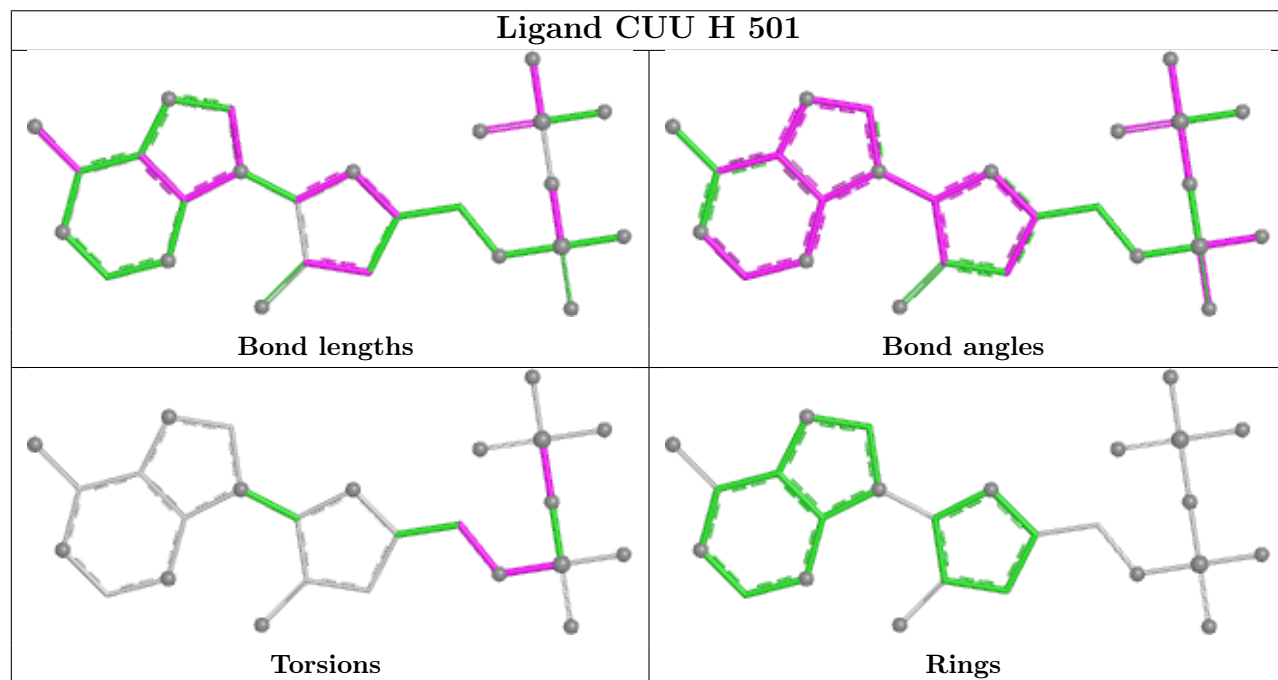
Ligand 3AT J 501

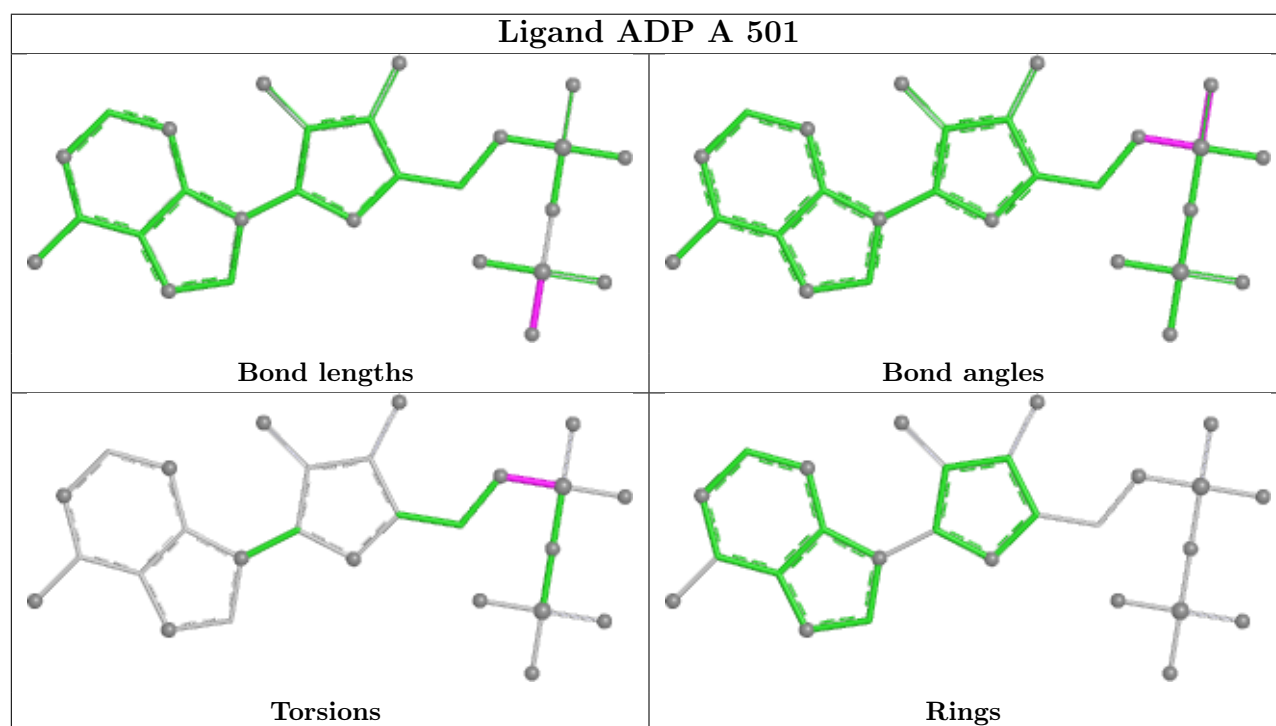
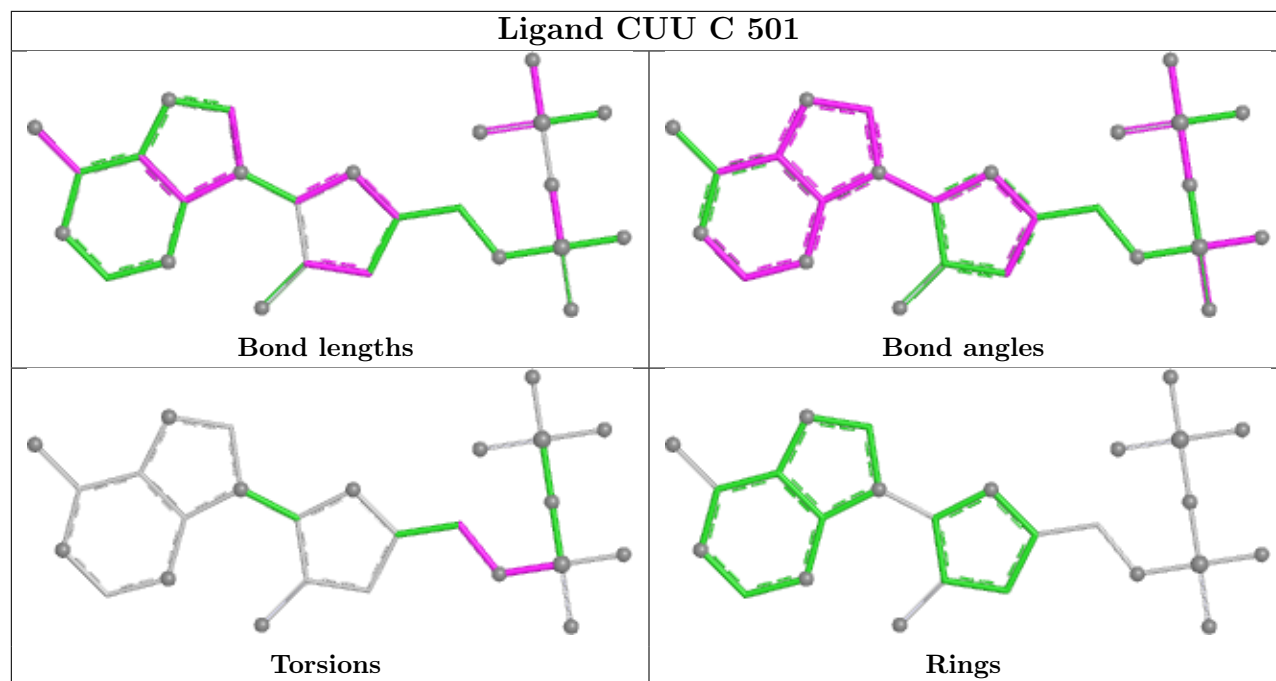


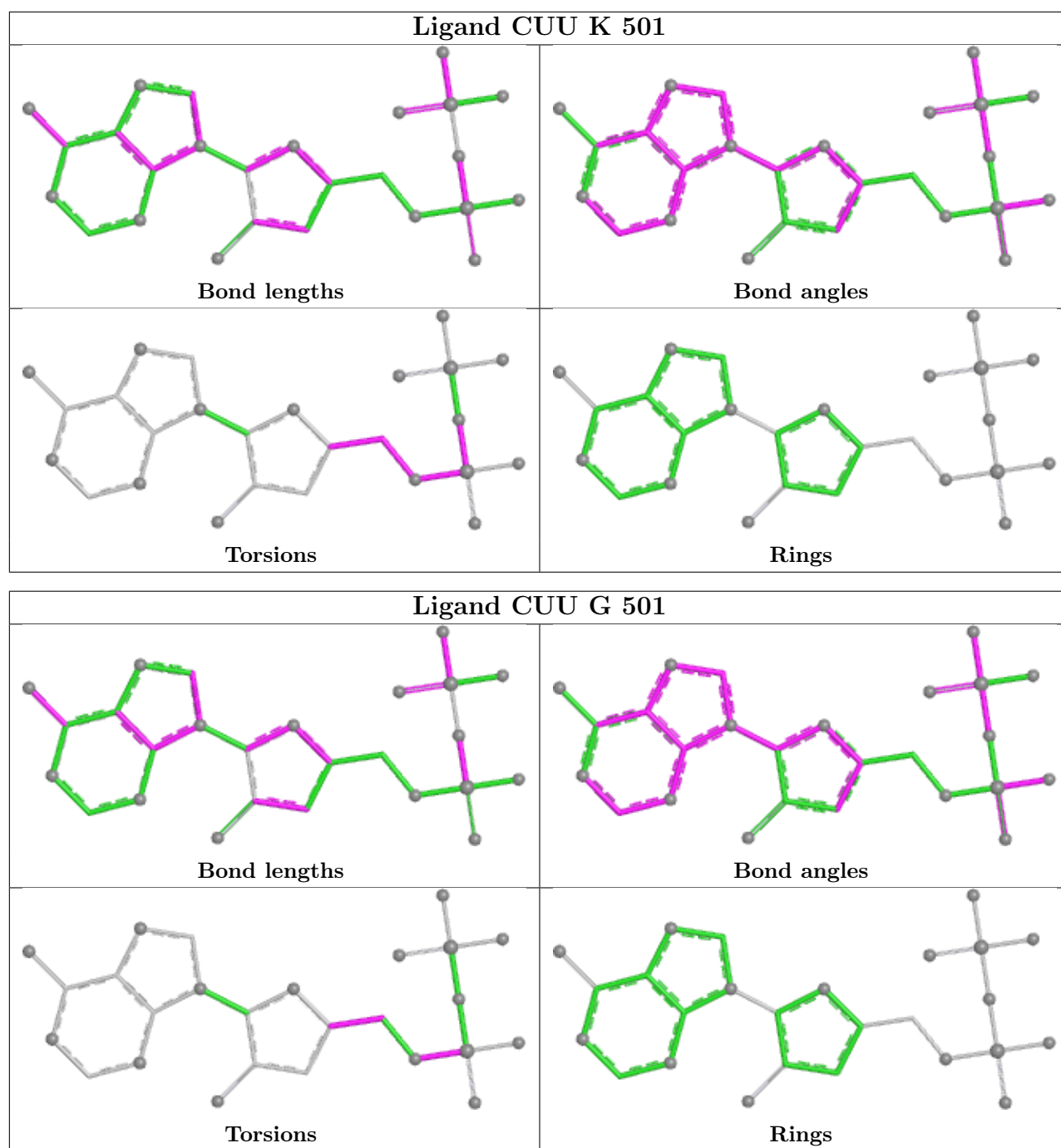
Ligand CU0 L 501



Ligand CUU H 501







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	316/355 (89%)	-1.08	0 100 100	34, 59, 100, 119	0
1	B	318/355 (89%)	-1.03	0 100 100	45, 68, 107, 116	0
1	C	313/355 (88%)	-1.05	0 100 100	44, 66, 98, 111	0
1	G	311/355 (87%)	-0.99	0 100 100	45, 70, 109, 139	0
1	H	318/355 (89%)	-1.08	0 100 100	47, 72, 97, 123	0
1	I	313/355 (88%)	-1.05	0 100 100	40, 64, 100, 124	0
2	D	303/366 (82%)	-1.04	0 100 100	49, 70, 103, 128	0
2	E	304/366 (83%)	-1.04	1 (0%) 90 87	42, 66, 108, 121	0
2	F	307/366 (83%)	-1.12	0 100 100	37, 62, 100, 120	0
2	J	302/366 (82%)	-1.02	0 100 100	46, 71, 120, 146	0
2	K	300/366 (81%)	-1.11	0 100 100	44, 67, 106, 120	0
2	L	300/366 (81%)	-1.03	0 100 100	49, 72, 117, 141	0
All	All	3705/4326 (85%)	-1.05	1 (0%) 100 100	34, 67, 107, 146	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	337	GLY	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

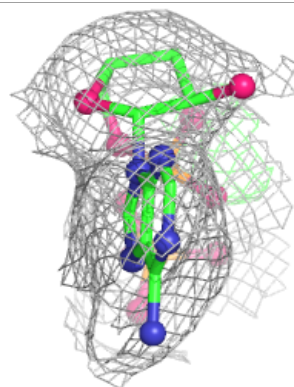
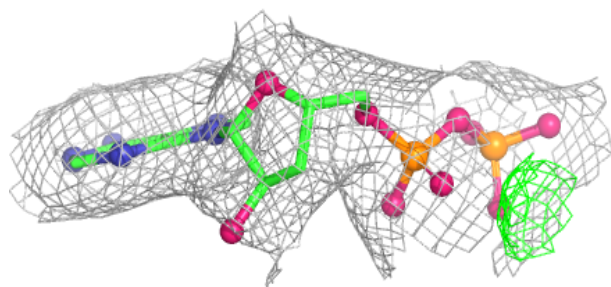
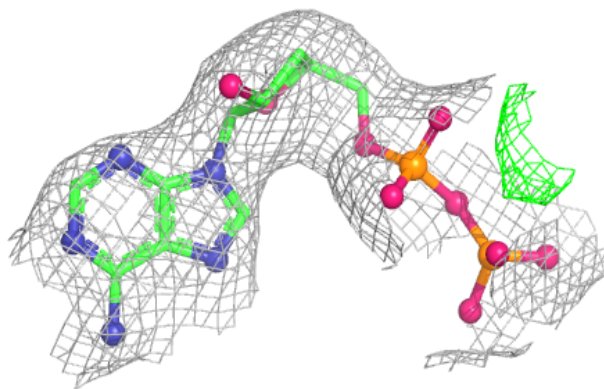
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CUU	B	501	26/26	0.98	0.04	56,57,67,68	0
5	MG	D	502	1/1	0.98	0.05	55,55,55,55	0
5	MG	L	502	1/1	0.98	0.04	56,56,56,56	0
6	3AT	E	501	30/30	0.98	0.04	64,66,68,68	0
4	CUU	F	501	26/26	0.99	0.03	61,63,65,65	0
4	CUU	G	501	26/26	0.99	0.05	54,59,76,76	0
4	CUU	H	501	26/26	0.99	0.03	68,72,74,75	0
4	CUU	I	501	26/26	0.99	0.04	44,47,50,51	0
4	CUU	K	501	26/26	0.99	0.04	75,77,78,79	0
3	ADP	A	501	27/27	0.99	0.03	38,48,51,52	0
4	CUU	C	501	26/26	0.99	0.04	51,62,63,64	0
4	CUU	D	501	26/26	0.99	0.04	76,77,78,78	0
6	3AT	J	501	30/30	0.99	0.04	79,83,95,95	0
7	CU0	L	501	17/17	0.99	0.03	58,65,67,67	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.

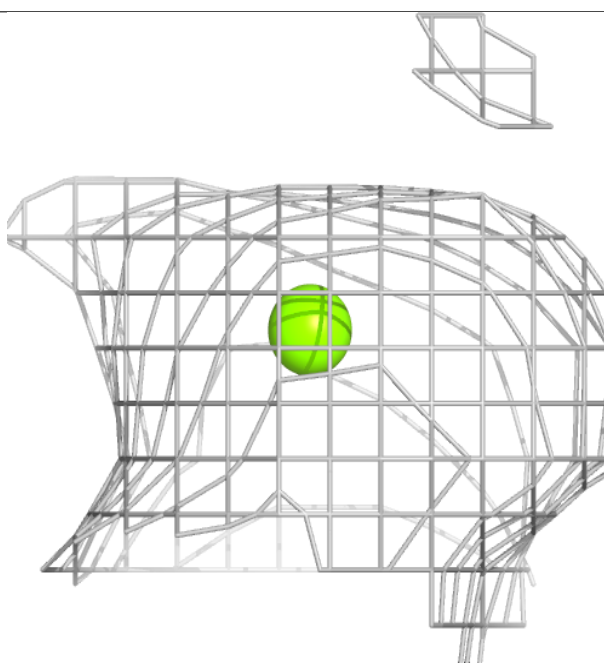
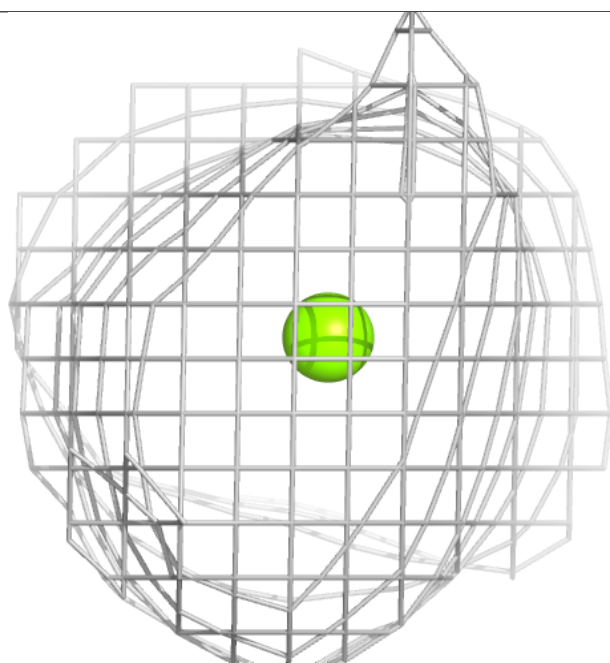
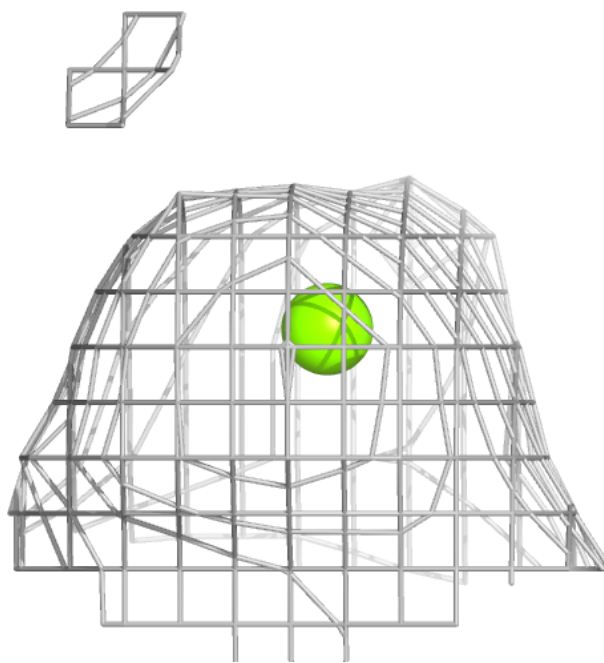
Electron density around CUU B 501:

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



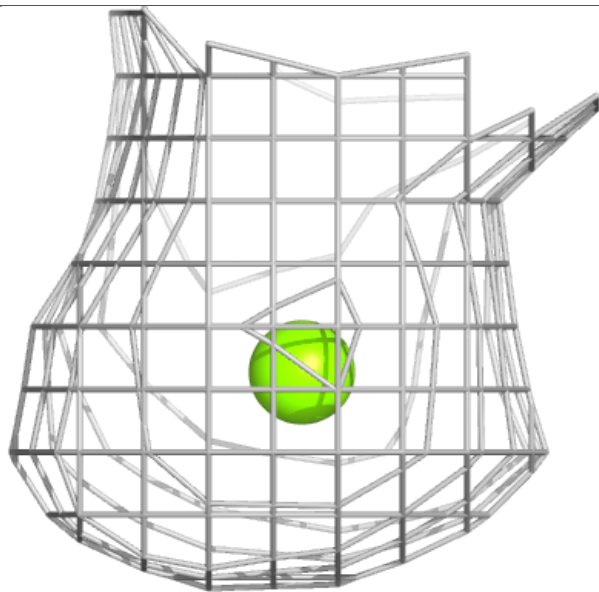
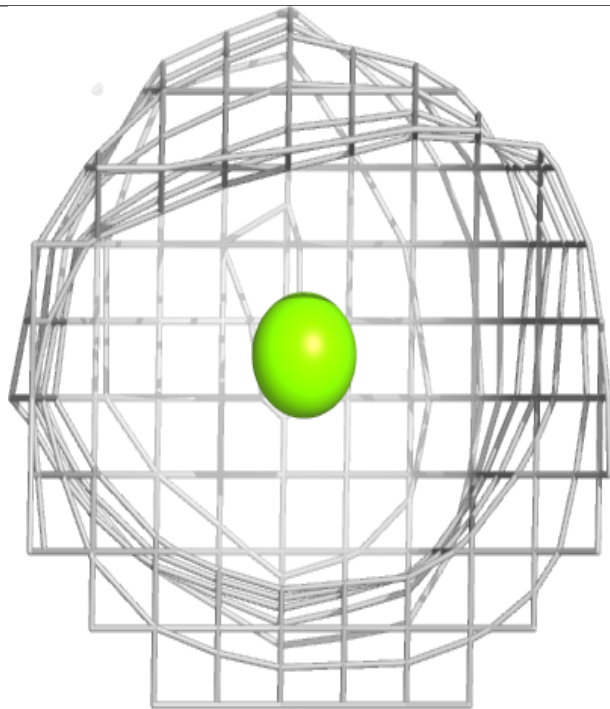
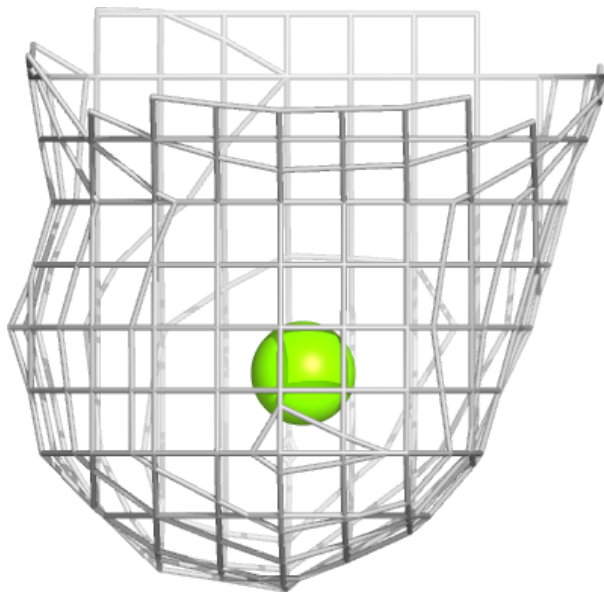
Electron density around MG D 502:

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



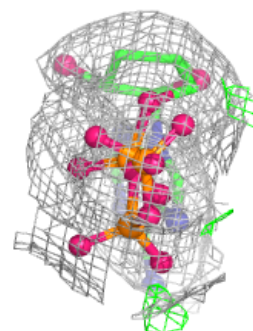
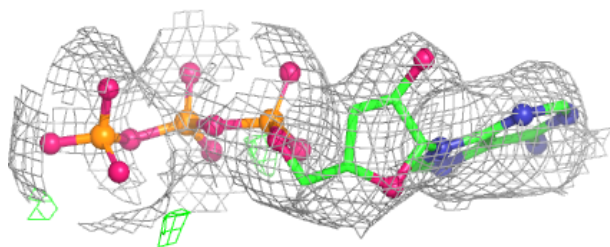
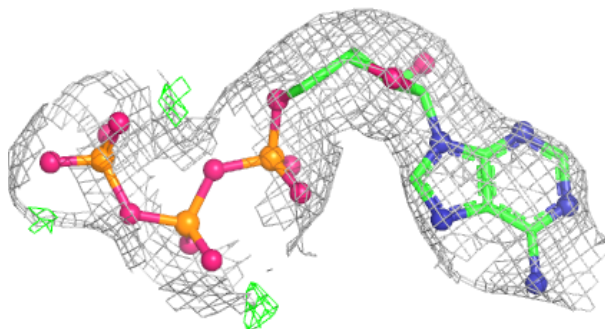
Electron density around MG L 502:

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and green (positive)

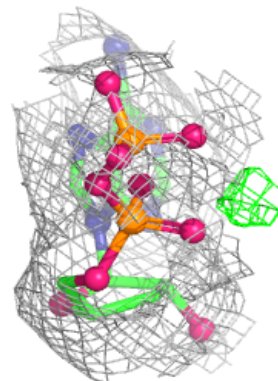
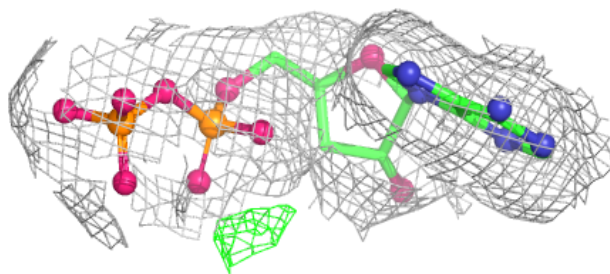
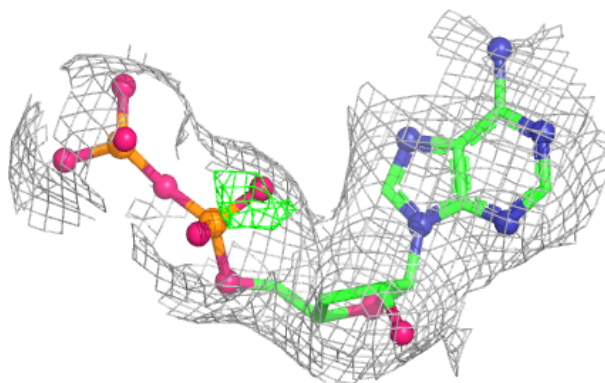


Electron density around 3AT E 501:

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

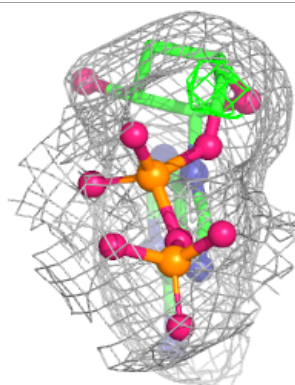
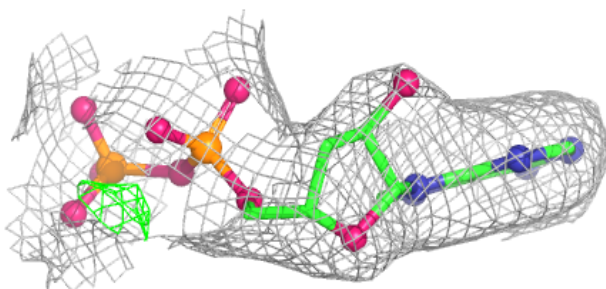
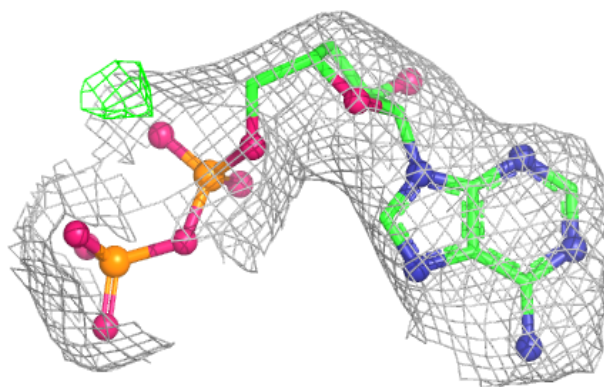
**Electron density around CUU F 501:**

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

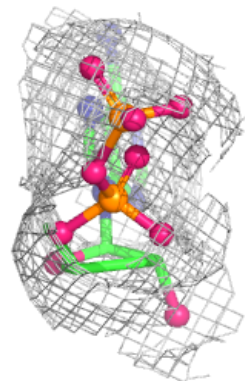
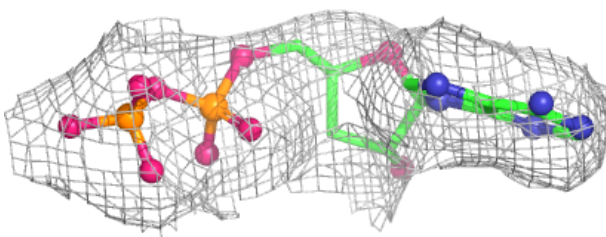
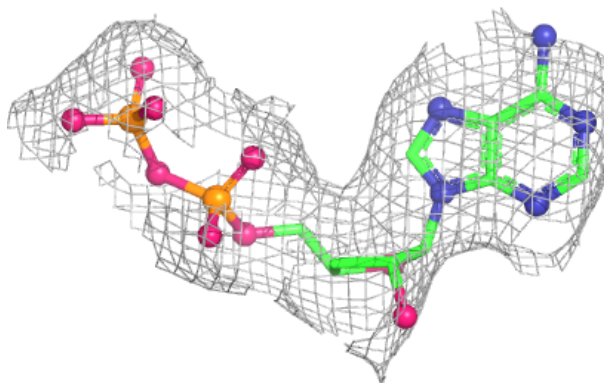


Electron density around CUU G 501:

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

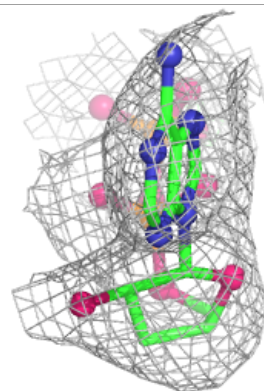
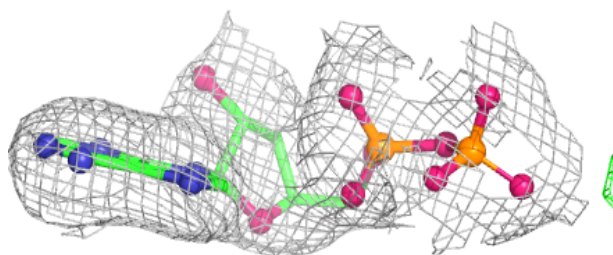
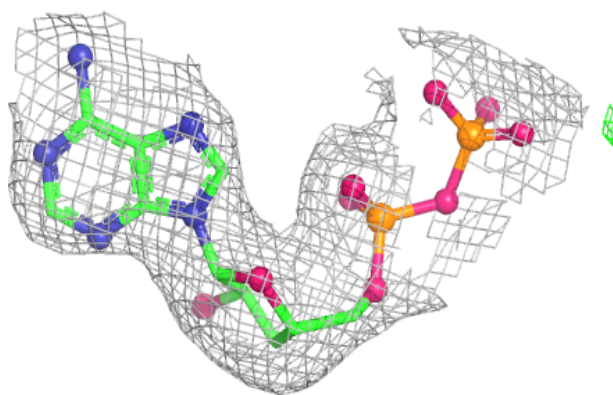
**Electron density around CUU H 501:**

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

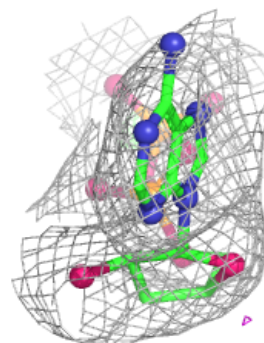
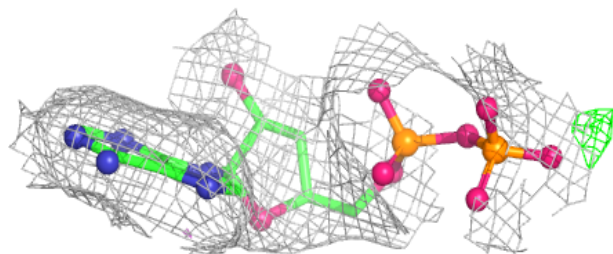
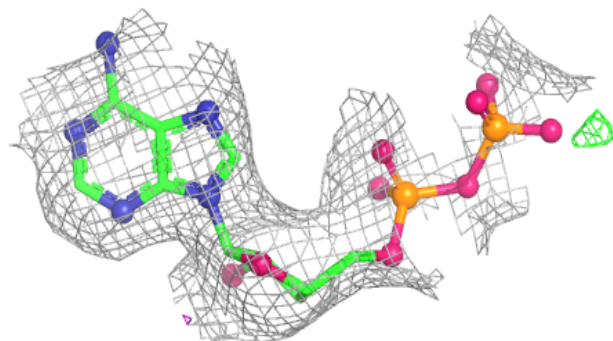


Electron density around CUU I 501:

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

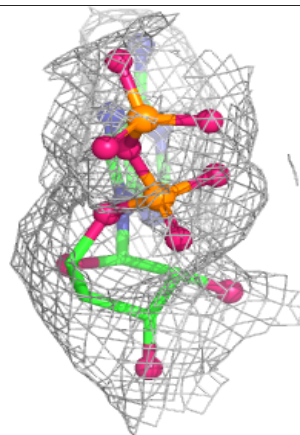
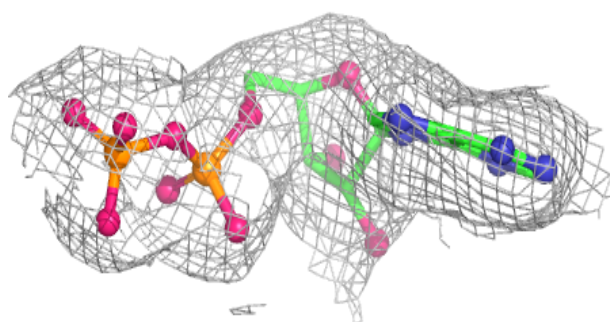
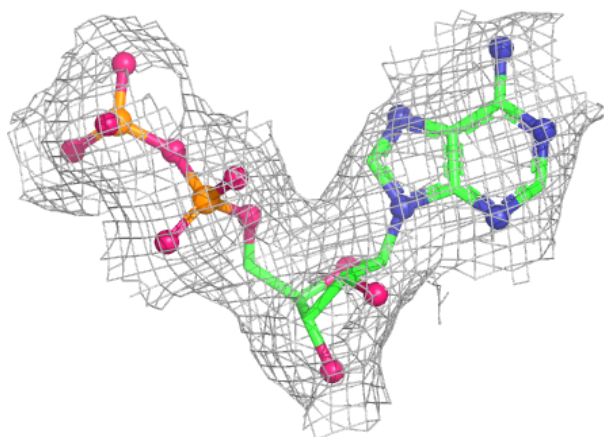
**Electron density around CUU K 501:**

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

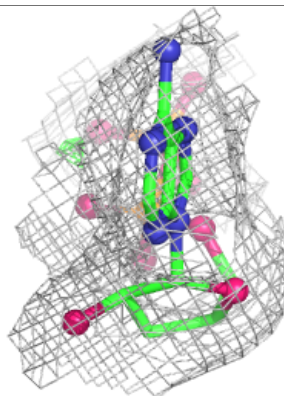
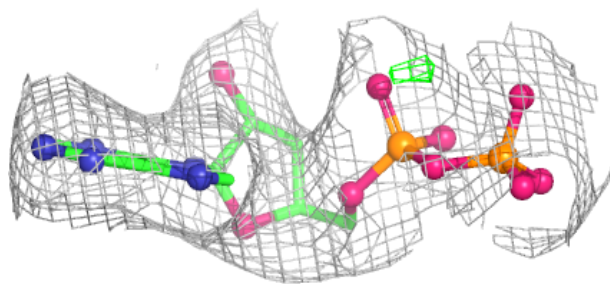
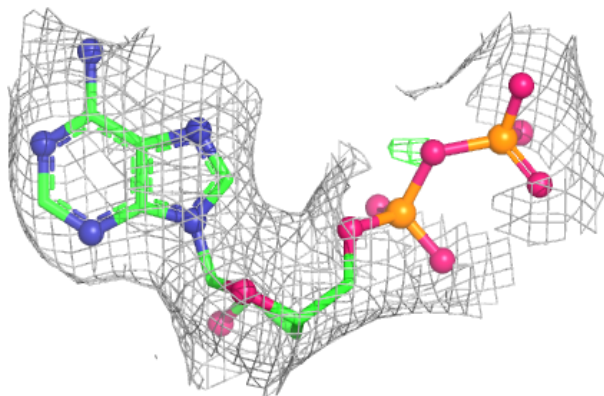


Electron density around ADP A 501:

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

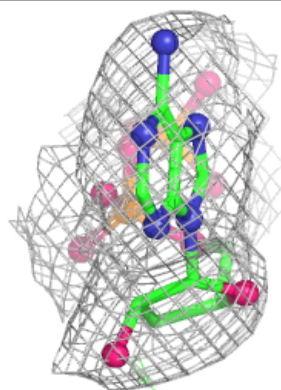
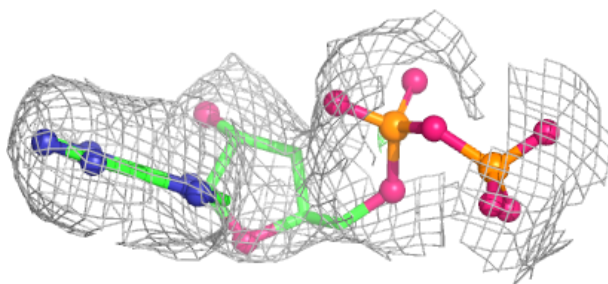
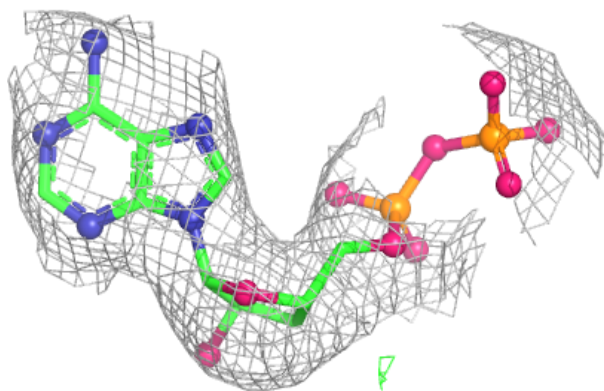
**Electron density around CUU C 501:**

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

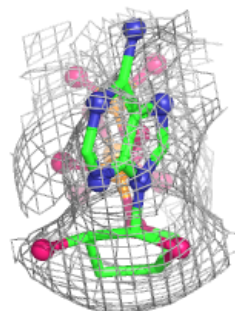
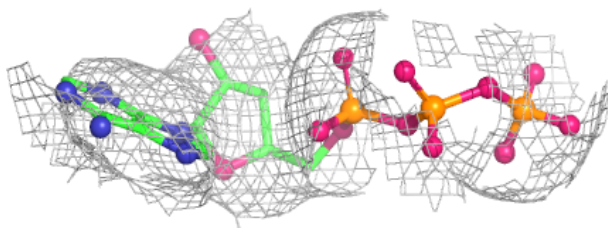
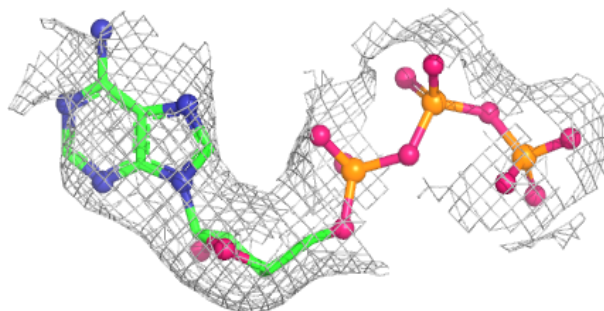


Electron density around CUU D 501:

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

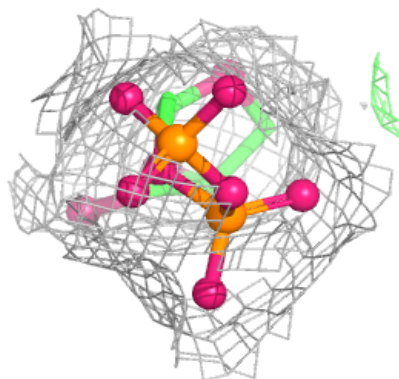
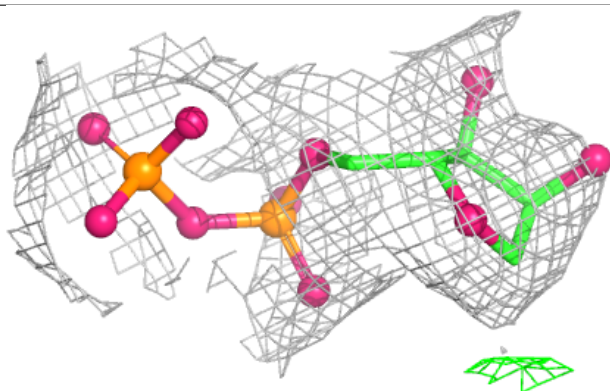
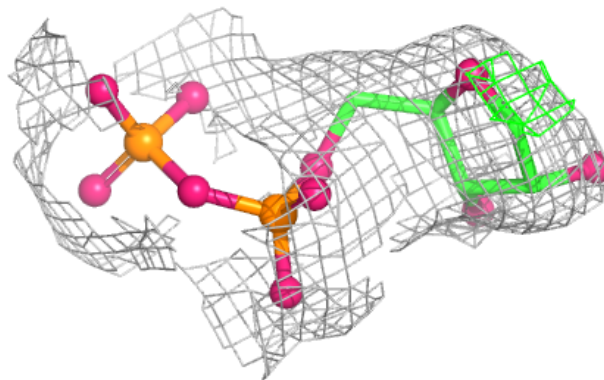
**Electron density around 3AT J 501:**

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



Electron density around CU0 L 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.