



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 12:28 AM EDT

PDB ID : 5Z2C  
Title : Crystal structure of ALPK-1 N-terminal domain in complex with ADP-heptose  
Authors : Ding, J.; She, Y.; Shao, F.  
Deposited on : 2018-01-02  
Resolution : 2.59 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

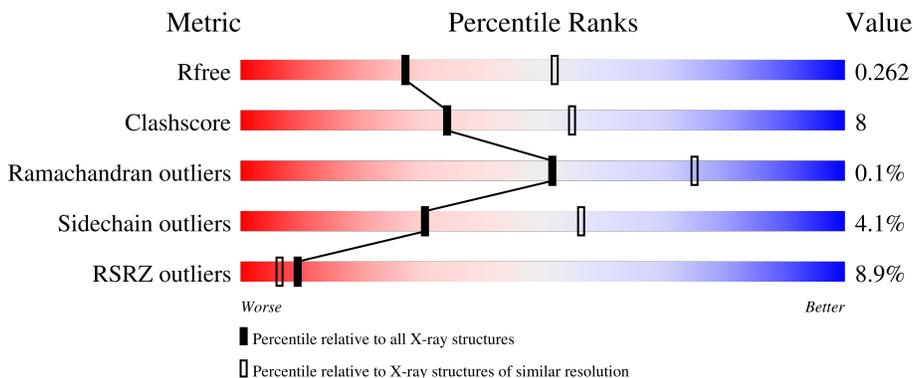
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	446	 86% 12%
1	B	446	 88% 11%
1	C	446	 78% 15%
1	D	446	 85% 12%
1	E	446	 84% 12%

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Mol	Chain	Length	Quality of chain
1	F	446	
1	G	446	
1	H	446	
1	I	446	

## 2 Entry composition [i](#)

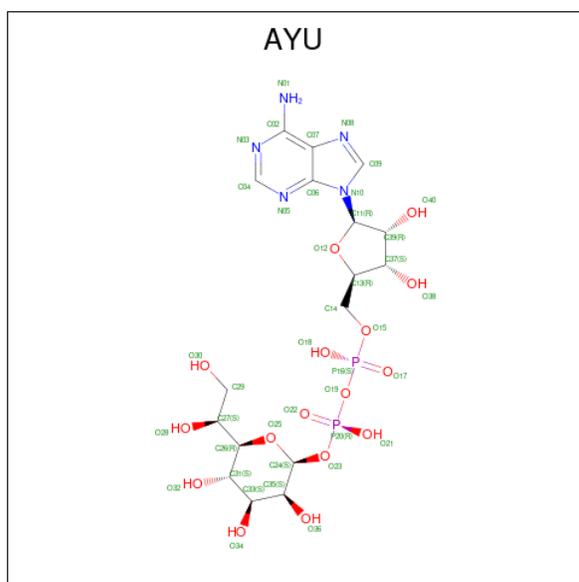
There are 2 unique types of molecules in this entry. The entry contains 30546 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	445	3469	2203	597	654	15	0	0	0
1	B	445	3469	2203	597	654	15	0	0	0
1	C	427	3324	2115	572	622	15	0	0	0
1	D	434	3388	2156	583	634	15	0	0	0
1	E	433	3378	2148	580	635	15	0	0	0
1	F	433	3379	2148	581	635	15	0	0	0
1	G	428	3327	2113	573	626	15	0	0	0
1	H	423	3284	2089	565	615	15	0	0	0
1	I	408	3168	2017	544	593	14	0	0	0

- Molecule 2 is [[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2S,3S,4S,5S,6R)-6-[(1S)-1,2-bis(oxidanyl)ethyl]-3,4,5-tris(oxidanyl)oxan-2-yl] hydrogen phosphate (three-letter code: AYU) (formula: C<sub>17</sub>H<sub>27</sub>N<sub>5</sub>O<sub>16</sub>P<sub>2</sub>).

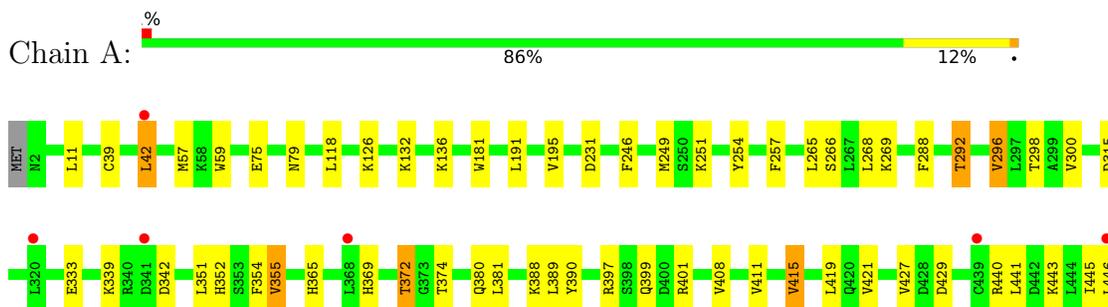


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			
2	A	1	Total	40	17	5	16	2	0	0
2	B	1	Total	40	17	5	16	2	0	0
2	C	1	Total	40	17	5	16	2	0	0
2	D	1	Total	40	17	5	16	2	0	0
2	E	1	Total	40	17	5	16	2	0	0
2	F	1	Total	40	17	5	16	2	0	0
2	G	1	Total	40	17	5	16	2	0	0
2	H	1	Total	40	17	5	16	2	0	0
2	I	1	Total	40	17	5	16	2	0	0

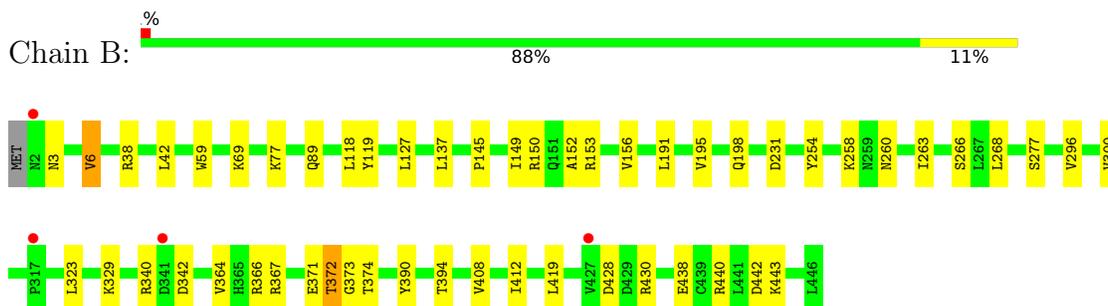
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

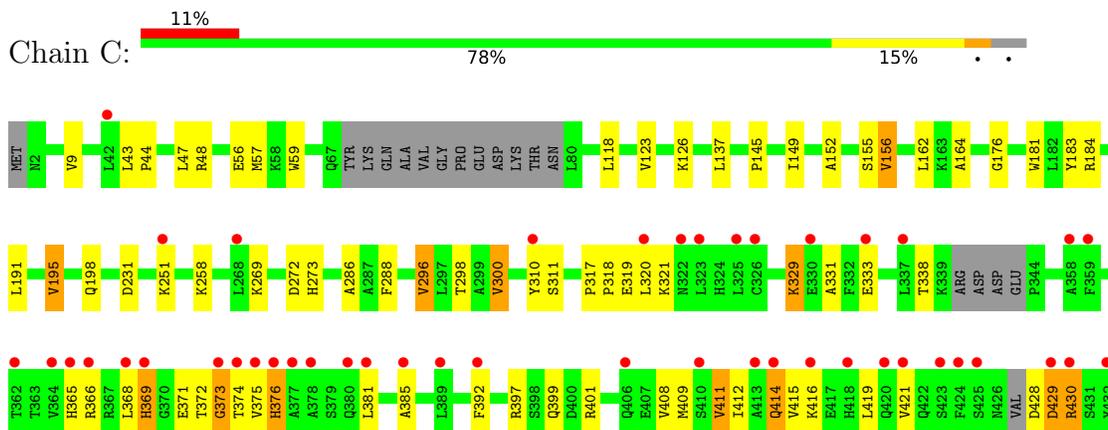
- Molecule 1: Alpha-protein kinase 1

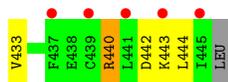


- Molecule 1: Alpha-protein kinase 1

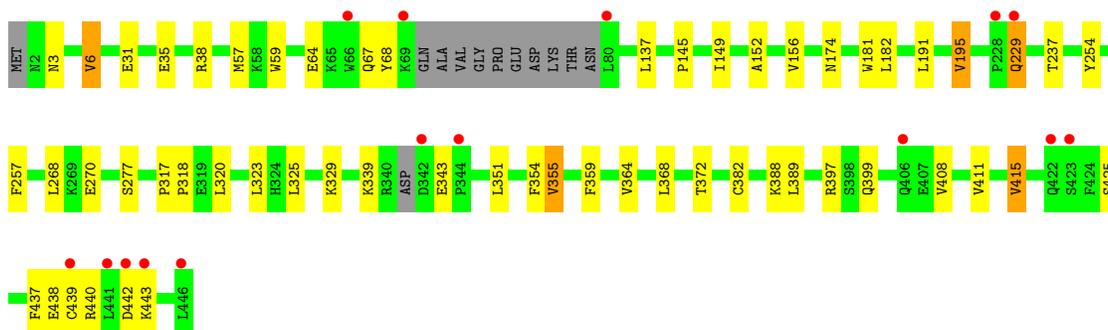
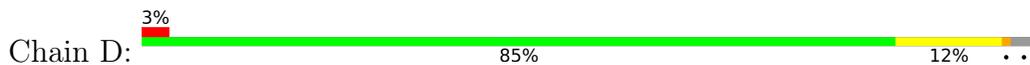


- Molecule 1: Alpha-protein kinase 1

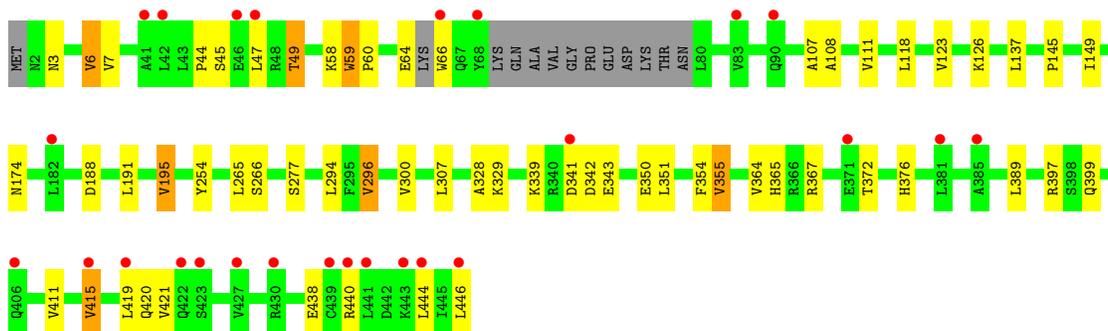
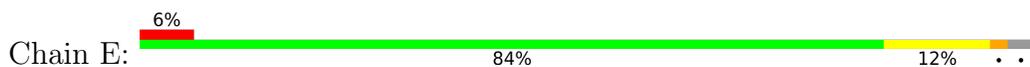




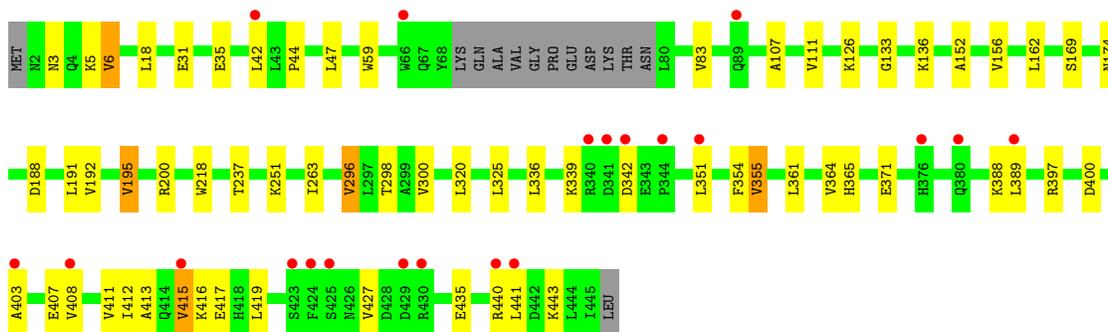
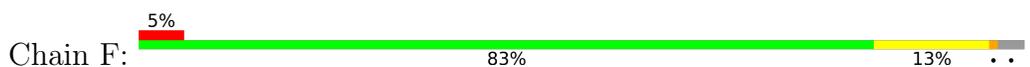
- Molecule 1: Alpha-protein kinase 1



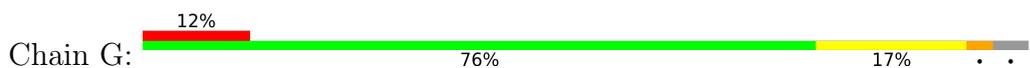
- Molecule 1: Alpha-protein kinase 1



- Molecule 1: Alpha-protein kinase 1



- Molecule 1: Alpha-protein kinase 1







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.26Å 214.39Å 173.15Å 90.00° 110.33° 90.00°	Depositor
Resolution (Å)	48.89 – 2.59 48.89 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.89-2.59) 93.1 (48.89-2.59)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.58Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.242 , 0.263 0.243 , 0.262	Depositor DCC
$R_{free}$ test set	2000 reflections (1.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.1	Xtrriage
Anisotropy	0.532	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	30546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: AYU

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	0.30	0/3528	0.44	0/4774
1	B	0.30	0/3528	0.46	0/4774
1	C	0.30	0/3378	0.48	0/4565
1	D	0.33	0/3444	0.44	0/4656
1	E	0.29	0/3434	0.44	0/4645
1	F	0.29	0/3436	0.43	0/4648
1	G	0.27	0/3380	0.42	0/4570
1	H	0.26	0/3336	0.44	0/4508
1	I	0.29	0/3220	0.44	0/4352
All	All	0.29	0/30684	0.44	0/41492

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3469	0	3541	44	0
1	B	3469	0	3541	29	0
1	C	3324	0	3402	82	0
1	D	3388	0	3467	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3378	0	3445	36	0
1	F	3379	0	3448	38	0
1	G	3327	0	3403	56	1
1	H	3284	0	3366	97	0
1	I	3168	0	3236	105	1
2	A	40	0	0	1	0
2	B	40	0	0	2	0
2	C	40	0	0	2	0
2	D	40	0	0	1	0
2	E	40	0	0	0	0
2	F	40	0	0	0	0
2	G	40	0	0	4	0
2	H	40	0	0	3	0
2	I	40	0	0	4	0
All	All	30546	0	30849	514	1

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 8.

The worst 5 of 514 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:H:424:PHE:HE1	1:H:434:PRO:CA	1.20	1.51
1:H:424:PHE:CE1	1:H:434:PRO:CG	1.94	1.51
1:I:366:ARG:CG	1:I:375:VAL:HG11	1.42	1.48
1:I:365:HIS:ND1	1:I:419:LEU:HD22	1.29	1.47
1:H:424:PHE:CE1	1:H:434:PRO:CA	2.03	1.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:ASN:O	1:I:262:GLN:NE2[2_11511]	2.17	0.03

## 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	443/446 (99%)	437 (99%)	6 (1%)	0	100	100
1	B	443/446 (99%)	436 (98%)	7 (2%)	0	100	100
1	C	419/446 (94%)	413 (99%)	4 (1%)	2 (0%)	29	52
1	D	428/446 (96%)	420 (98%)	8 (2%)	0	100	100
1	E	427/446 (96%)	420 (98%)	6 (1%)	1 (0%)	47	71
1	F	429/446 (96%)	422 (98%)	7 (2%)	0	100	100
1	G	422/446 (95%)	413 (98%)	8 (2%)	1 (0%)	47	71
1	H	415/446 (93%)	406 (98%)	9 (2%)	0	100	100
1	I	398/446 (89%)	394 (99%)	3 (1%)	1 (0%)	41	64
All	All	3824/4014 (95%)	3761 (98%)	58 (2%)	5 (0%)	51	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	429	ASP
1	E	420	GLN
1	I	338	THR
1	C	373	GLY
1	G	370	GLY

### 5.3.2 Protein sidechains [i](#)

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	382/383 (100%)	371 (97%)	11 (3%)	42	68
1	B	382/383 (100%)	372 (97%)	10 (3%)	46	72
1	C	366/383 (96%)	348 (95%)	18 (5%)	25	48
1	D	373/383 (97%)	363 (97%)	10 (3%)	44	71
1	E	372/383 (97%)	360 (97%)	12 (3%)	39	65
1	F	372/383 (97%)	358 (96%)	14 (4%)	33	59
1	G	367/383 (96%)	345 (94%)	22 (6%)	19	39
1	H	362/383 (94%)	338 (93%)	24 (7%)	16	33
1	I	347/383 (91%)	332 (96%)	15 (4%)	29	54
All	All	3323/3447 (96%)	3187 (96%)	136 (4%)	30	56

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	368	LEU
1	H	433	VAL
1	I	386	MET
1	D	439	CYS
1	D	415	VAL

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

Mol	Chain	Res	Type
1	C	322	ASN
1	C	376	HIS
1	C	414	GLN
1	D	174	ASN
1	H	426	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 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	AYU	H	501	-	37,43,43	2.73	15 (40%)	47,66,66	1.68	8 (17%)
2	AYU	F	501	-	37,43,43	2.45	12 (32%)	47,66,66	1.47	8 (17%)
2	AYU	B	501	-	37,43,43	2.55	13 (35%)	47,66,66	1.36	5 (10%)
2	AYU	I	501	-	37,43,43	2.65	16 (43%)	47,66,66	1.59	7 (14%)
2	AYU	E	501	-	37,43,43	2.69	13 (35%)	47,66,66	1.49	7 (14%)
2	AYU	G	501	-	37,43,43	2.65	14 (37%)	47,66,66	1.55	8 (17%)
2	AYU	C	501	-	37,43,43	2.58	15 (40%)	47,66,66	1.51	8 (17%)
2	AYU	D	501	-	37,43,43	2.44	13 (35%)	47,66,66	1.46	7 (14%)
2	AYU	A	501	-	37,43,43	2.57	13 (35%)	47,66,66	1.52	6 (12%)

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	AYU	H	501	-	-	1/23/63/63	0/4/4/4
2	AYU	F	501	-	-	1/23/63/63	0/4/4/4
2	AYU	B	501	-	-	1/23/63/63	0/4/4/4
2	AYU	I	501	-	-	1/23/63/63	0/4/4/4
2	AYU	E	501	-	-	0/23/63/63	0/4/4/4
2	AYU	G	501	-	-	1/23/63/63	0/4/4/4
2	AYU	C	501	-	-	1/23/63/63	0/4/4/4
2	AYU	D	501	-	-	0/23/63/63	0/4/4/4
2	AYU	A	501	-	-	1/23/63/63	0/4/4/4

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	AYU	P20-O23	9.89	1.86	1.60
2	E	501	AYU	P20-O23	9.83	1.86	1.60
2	G	501	AYU	P20-O23	9.61	1.85	1.60
2	C	501	AYU	P20-O23	9.08	1.84	1.60
2	A	501	AYU	P20-O23	8.99	1.84	1.60

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	AYU	C27-C26-C31	-4.58	106.43	114.03
2	G	501	AYU	C27-C26-C31	-4.50	106.56	114.03
2	I	501	AYU	C27-C26-C31	-4.50	106.56	114.03
2	E	501	AYU	O19-P20-O23	4.11	110.78	102.48
2	C	501	AYU	C27-C26-C31	-4.09	107.24	114.03

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	AYU	C35-C24-O23-P20
2	F	501	AYU	C35-C24-O23-P20
2	H	501	AYU	C35-C24-O23-P20
2	C	501	AYU	C35-C24-O23-P20
2	I	501	AYU	C35-C24-O23-P20

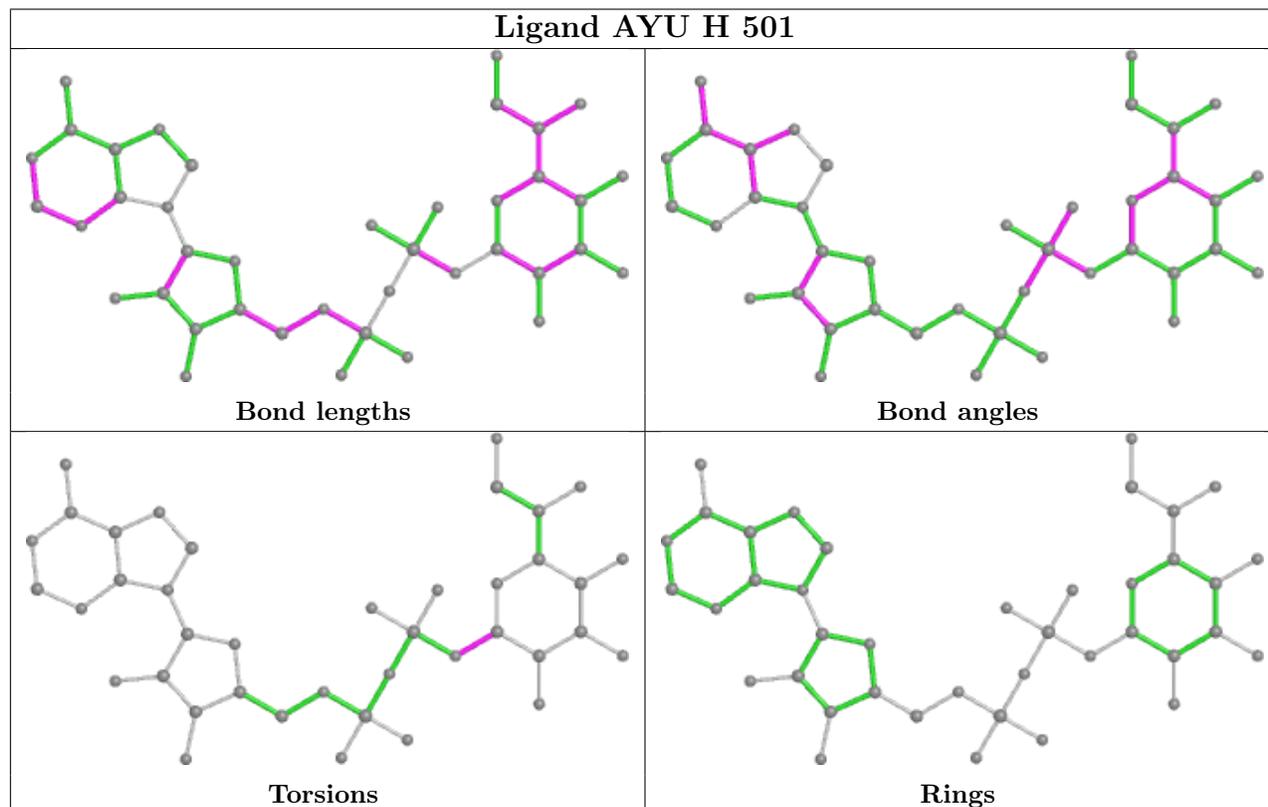
There are no ring outliers.

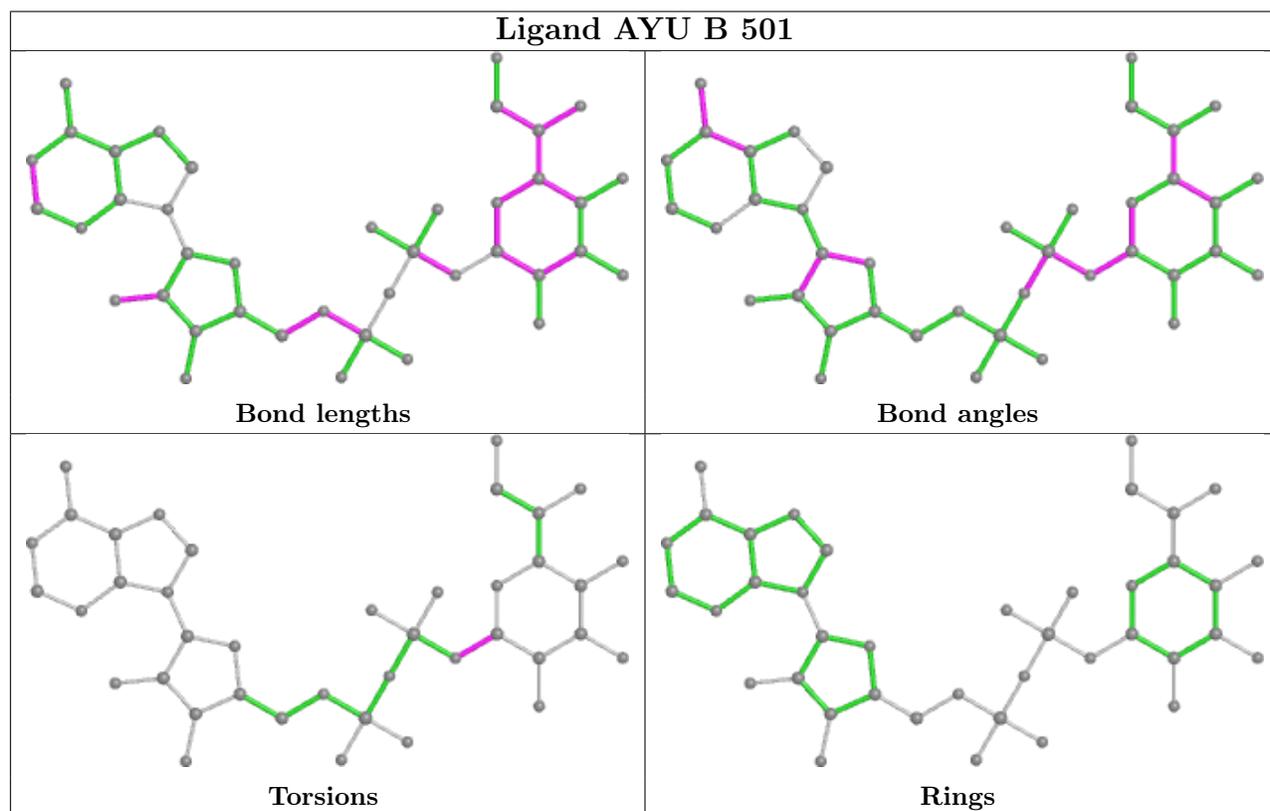
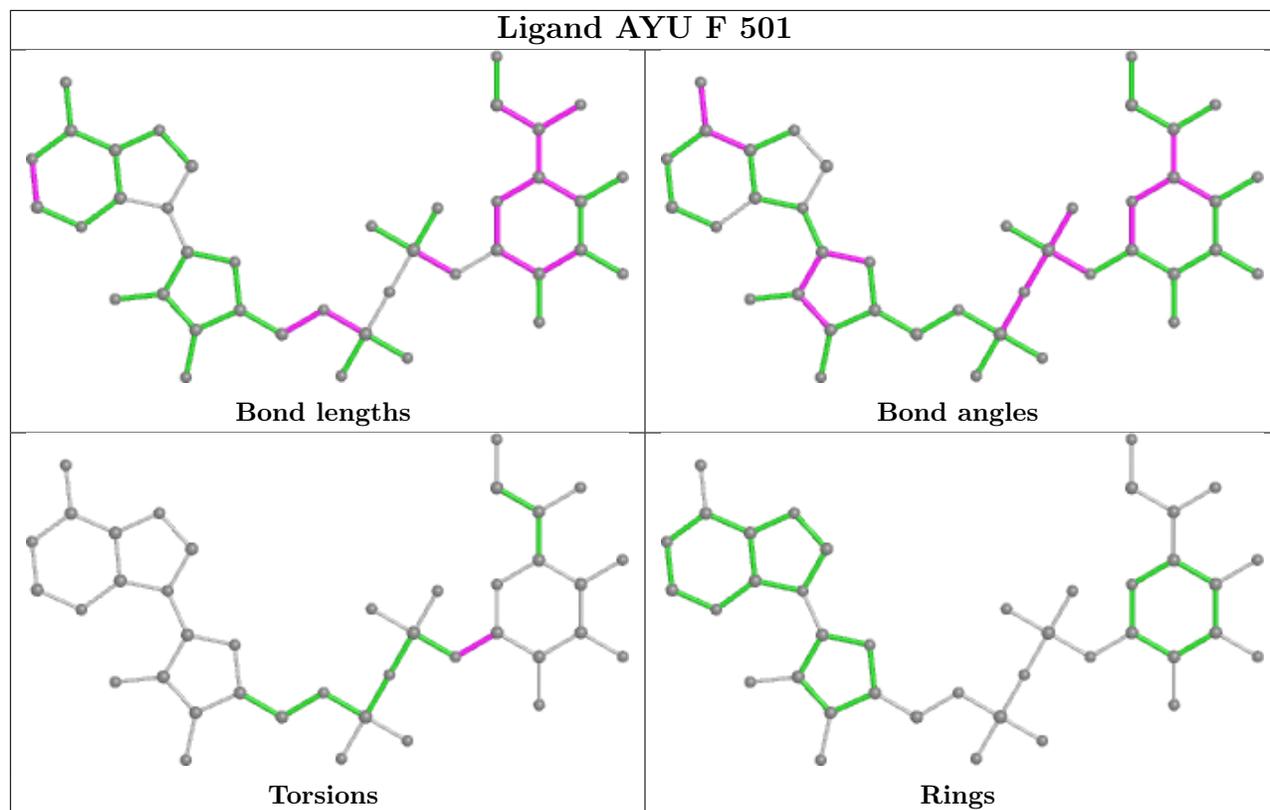
7 monomers are involved in 17 short contacts:

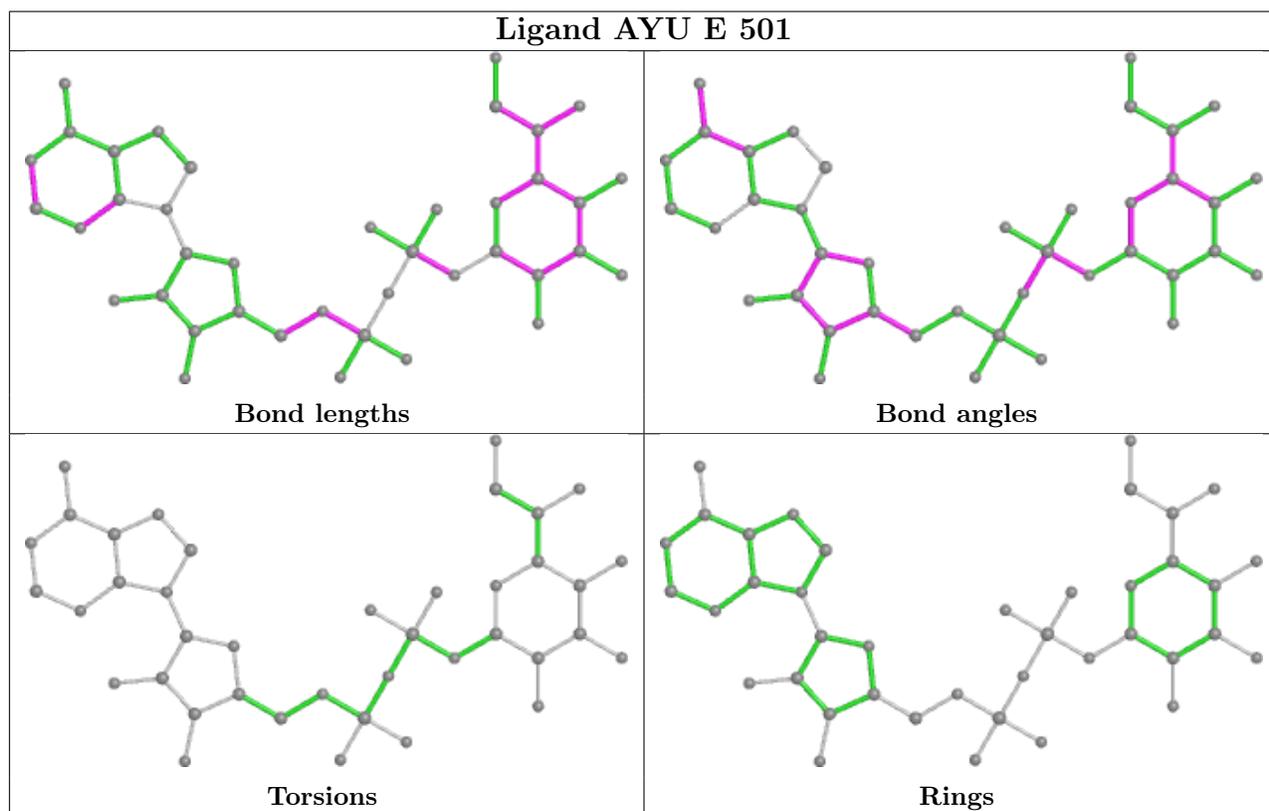
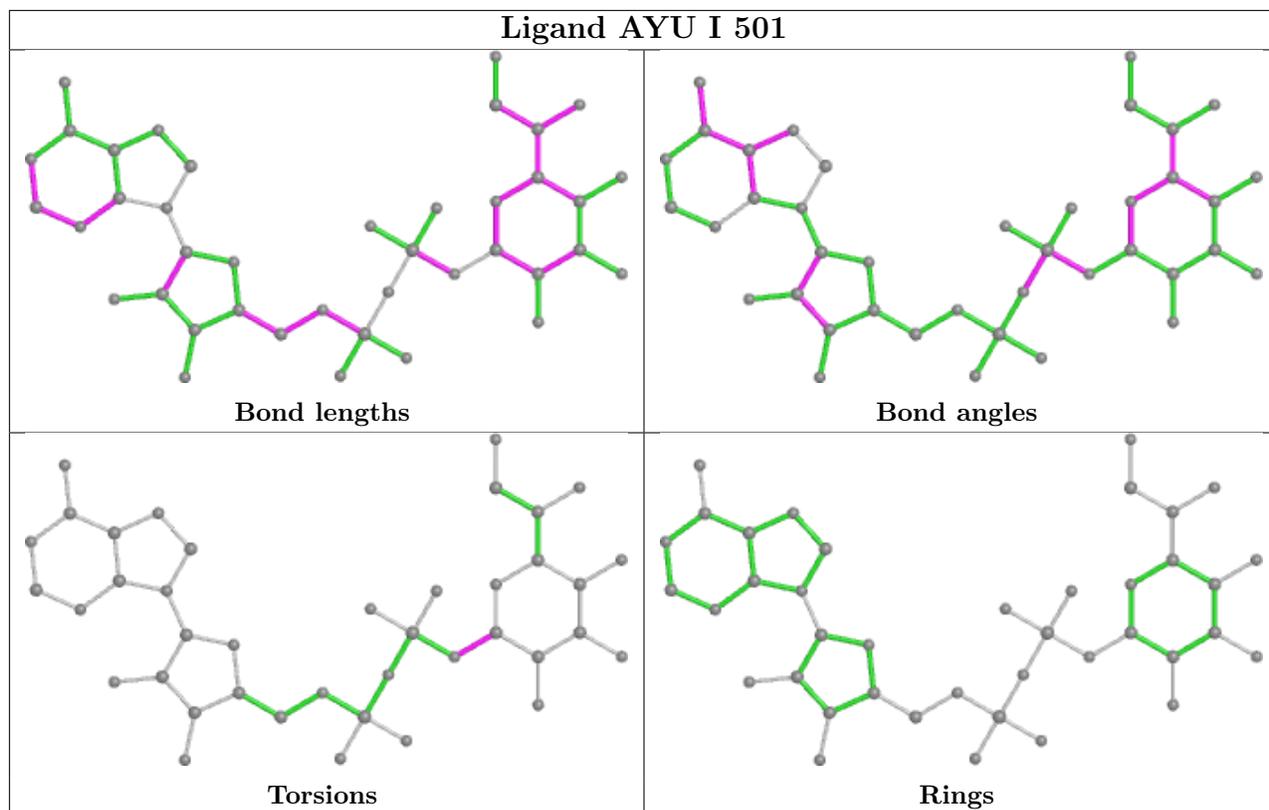
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	AYU	3	0
2	B	501	AYU	2	0
2	I	501	AYU	4	0
2	G	501	AYU	4	0
2	C	501	AYU	2	0
2	D	501	AYU	1	0
2	A	501	AYU	1	0

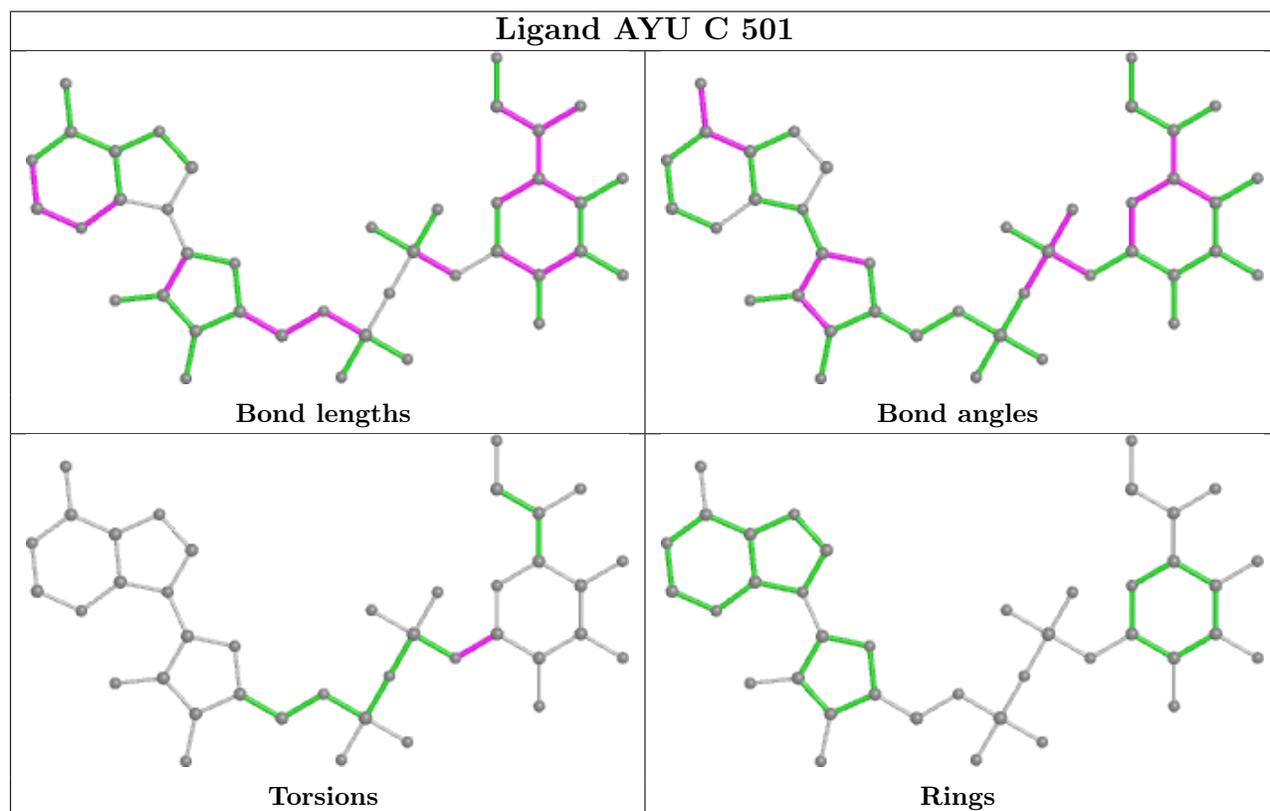
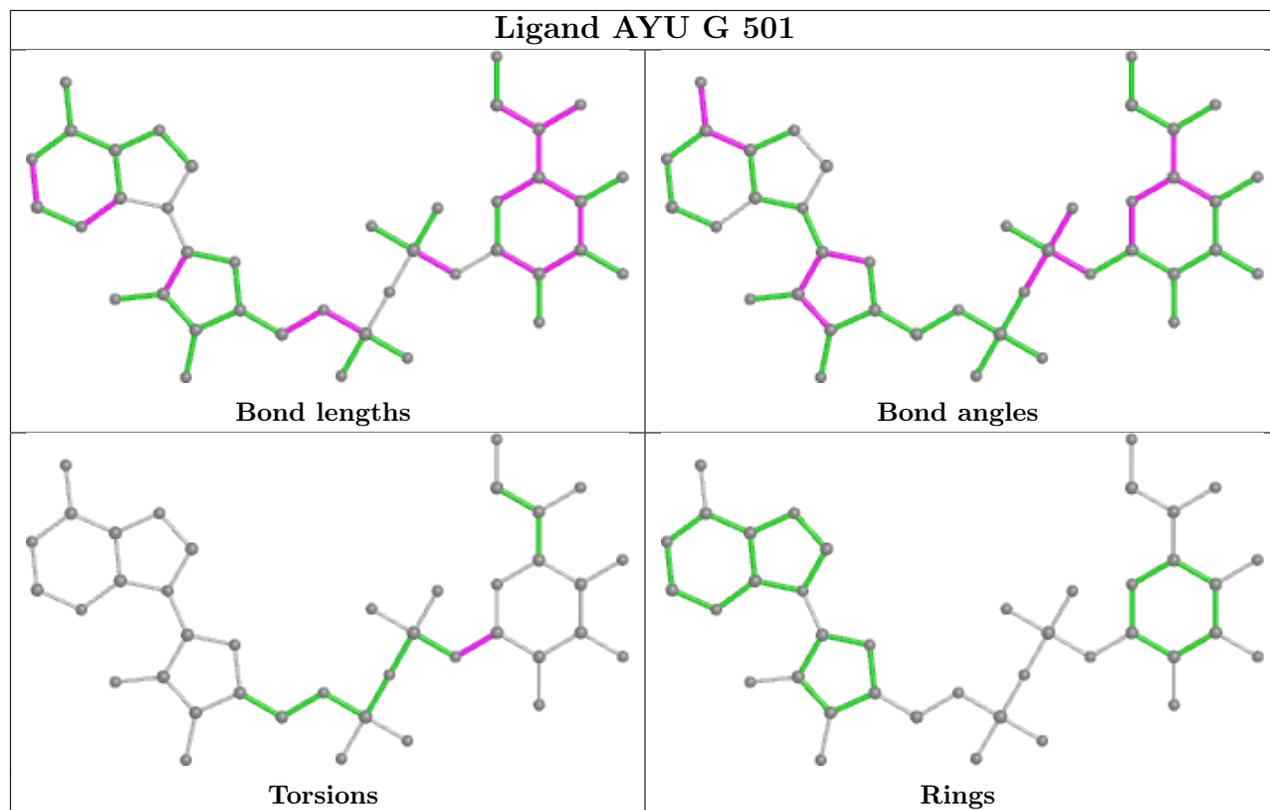
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

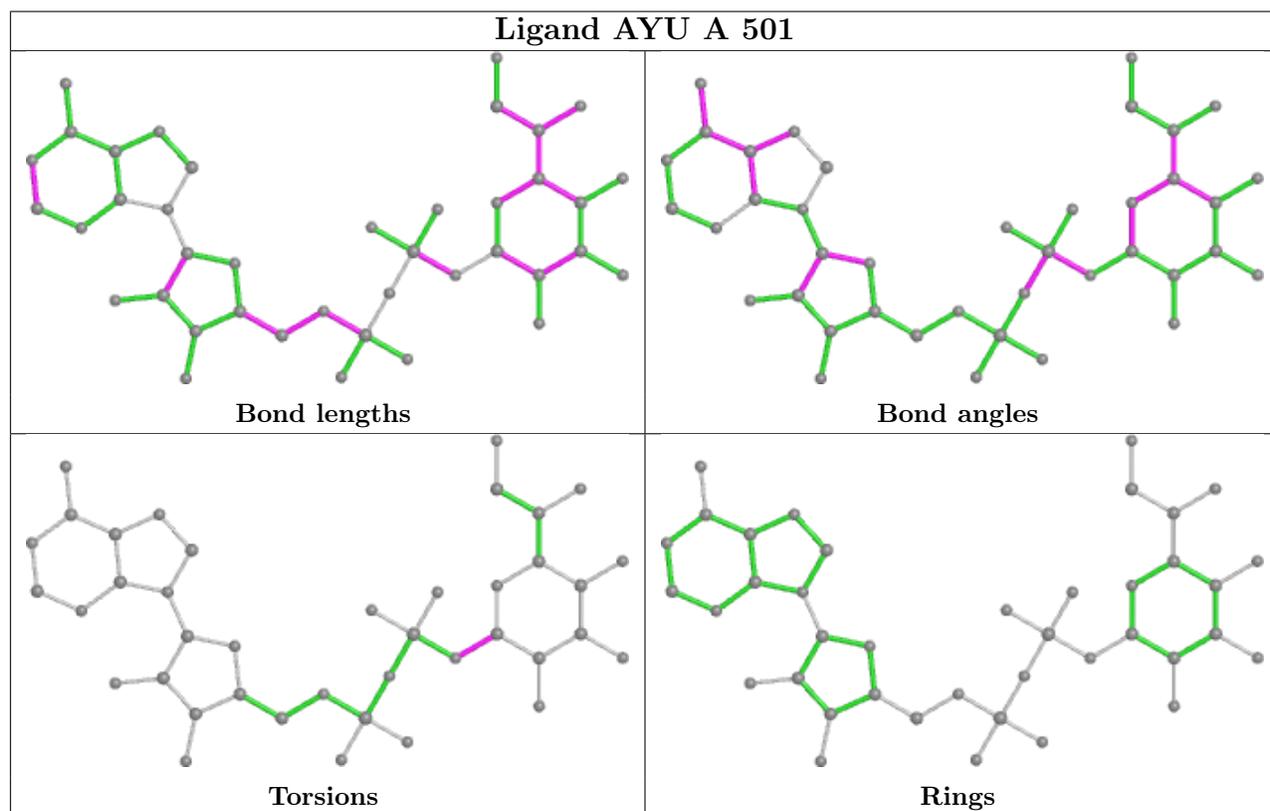
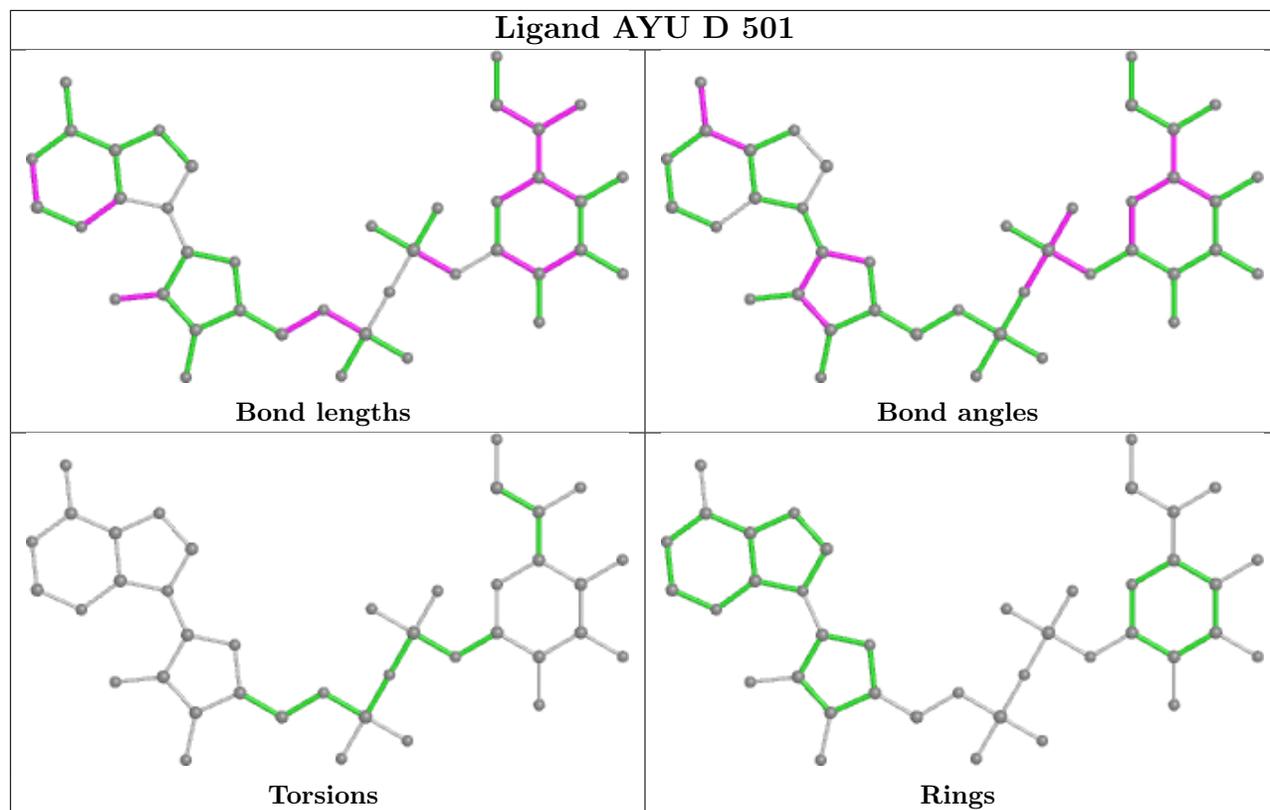
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	445/446 (99%)	0.31	6 (1%) 77 73	26, 41, 77, 119	0
1	B	445/446 (99%)	0.14	4 (0%) 84 82	25, 38, 67, 111	0
1	C	427/446 (95%)	0.76	50 (11%) 4 3	31, 59, 113, 138	0
1	D	434/446 (97%)	0.29	15 (3%) 44 36	26, 44, 74, 116	0
1	E	433/446 (97%)	0.52	26 (6%) 21 16	26, 48, 84, 116	0
1	F	433/446 (97%)	0.40	21 (4%) 30 24	26, 52, 83, 112	0
1	G	428/446 (95%)	0.91	55 (12%) 3 2	45, 70, 102, 126	0
1	H	423/446 (94%)	1.29	91 (21%) 0 0	51, 96, 128, 152	0
1	I	408/446 (91%)	1.02	76 (18%) 1 0	36, 78, 139, 180	0
All	All	3876/4014 (96%)	0.62	344 (8%) 9 6	25, 56, 114, 180	0

The worst 5 of 344 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	378	ALA	7.3
1	A	341	ASP	6.4
1	C	413	ALA	5.8
1	I	276	LEU	5.7
1	C	323	LEU	5.5

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

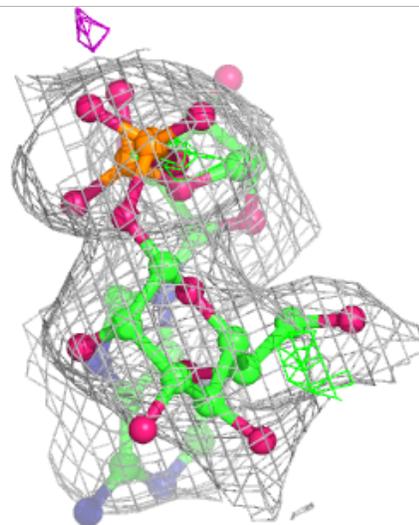
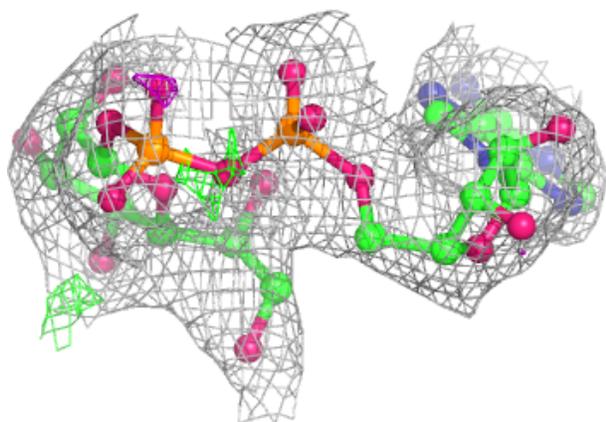
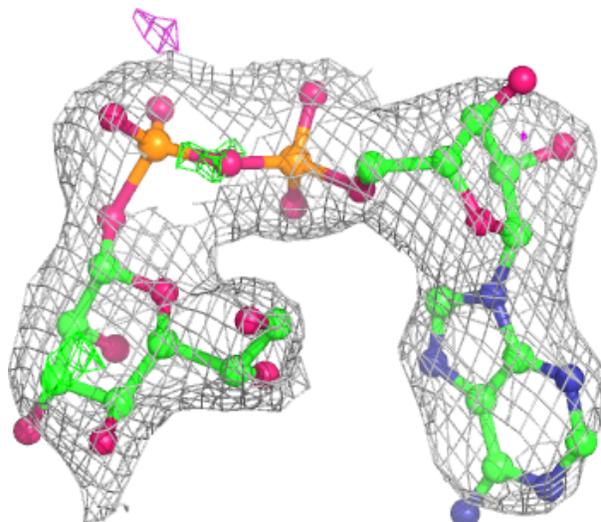
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	AYU	H	501	40/40	0.92	0.19	79,86,90,94	0
2	AYU	G	501	40/40	0.94	0.18	52,58,65,71	0
2	AYU	C	501	40/40	0.95	0.19	32,43,57,63	0
2	AYU	I	501	40/40	0.95	0.18	57,70,86,99	0
2	AYU	F	501	40/40	0.96	0.16	34,40,43,50	0
2	AYU	A	501	40/40	0.96	0.20	26,30,37,43	0
2	AYU	D	501	40/40	0.97	0.17	25,31,35,45	0
2	AYU	E	501	40/40	0.97	0.17	30,36,40,53	0
2	AYU	B	501	40/40	0.97	0.17	19,28,33,35	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.

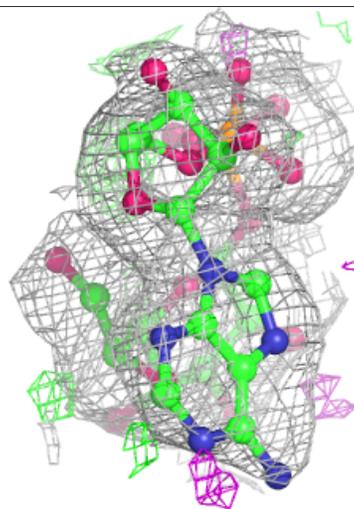
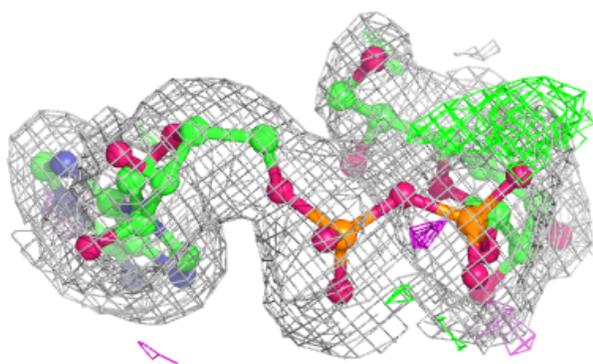
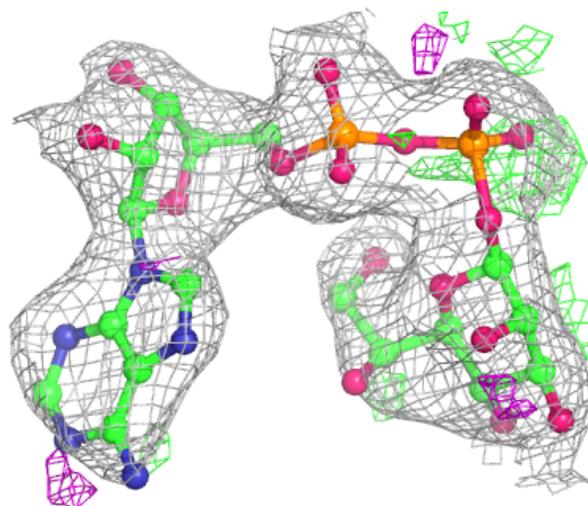
**Electron density around AYU H 501:**

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



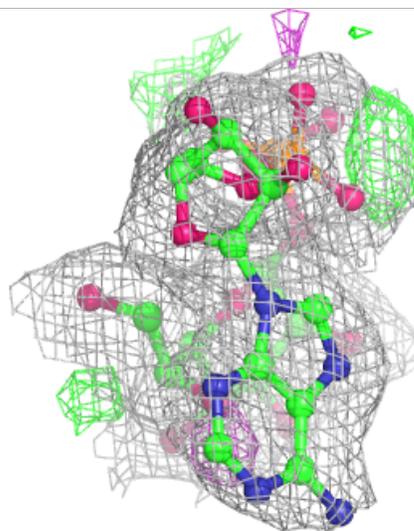
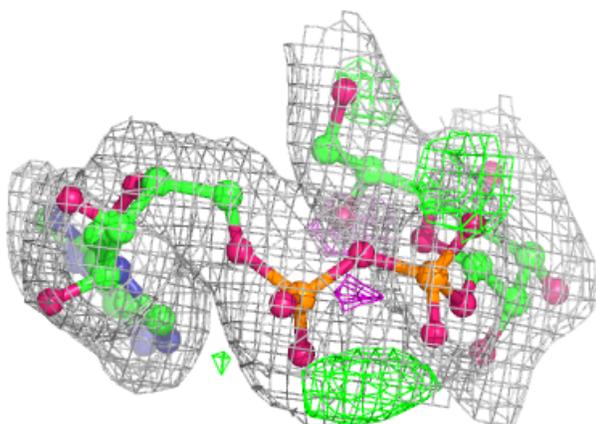
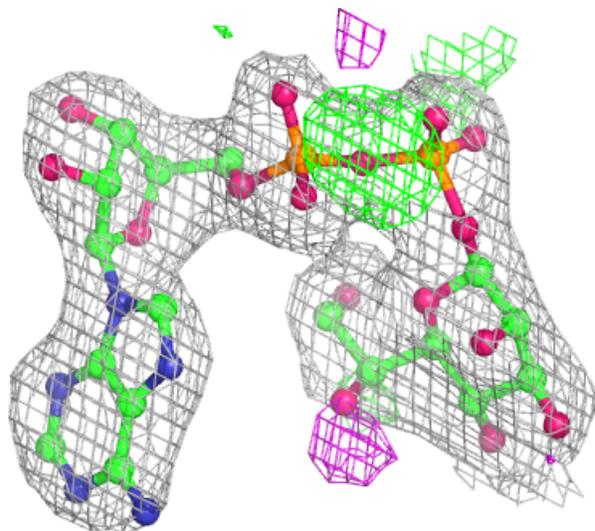
**Electron density around AYU G 501:**

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



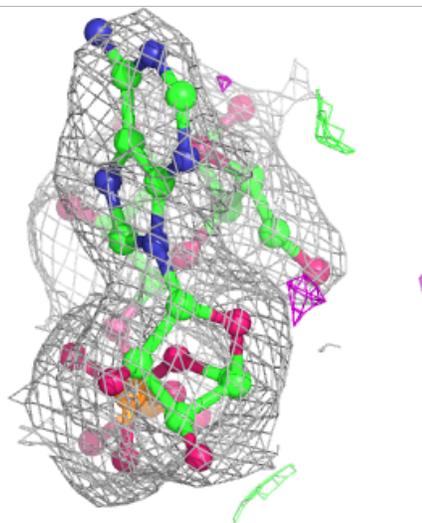
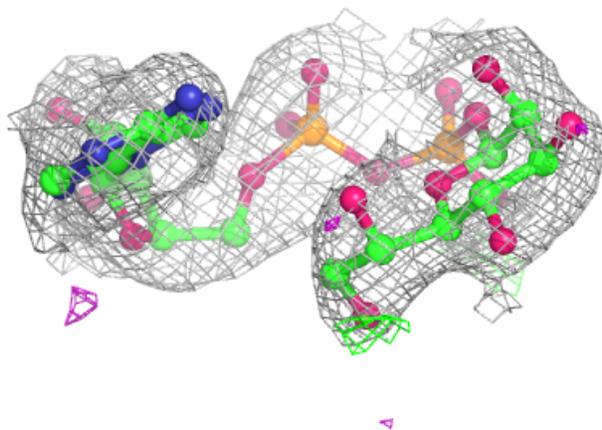
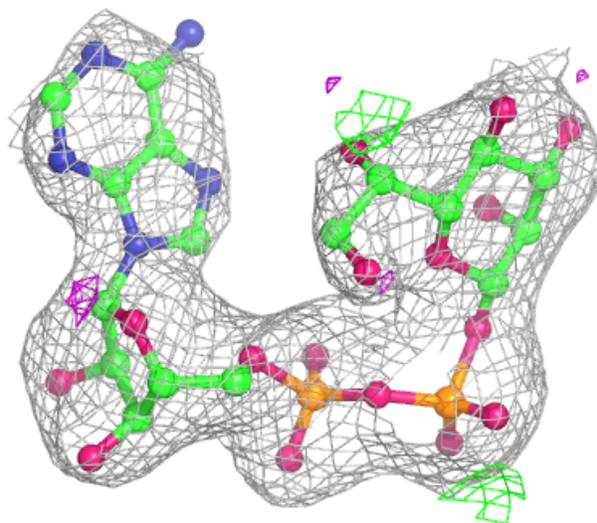
**Electron density around AYU C 501:**

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



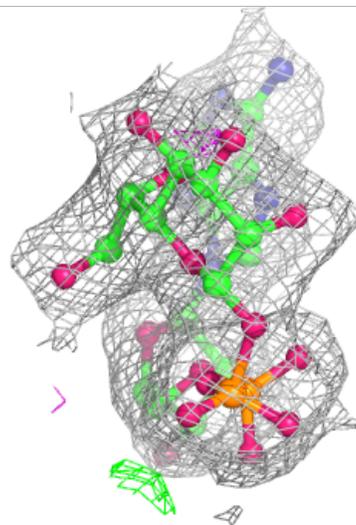
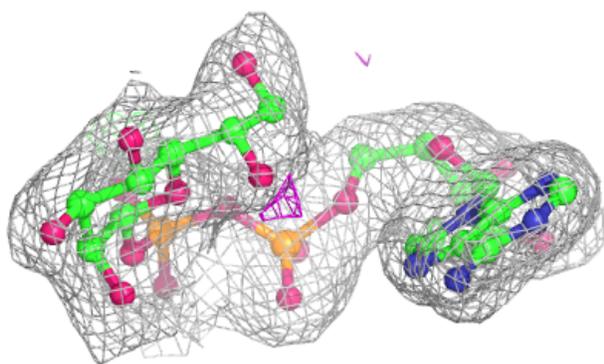
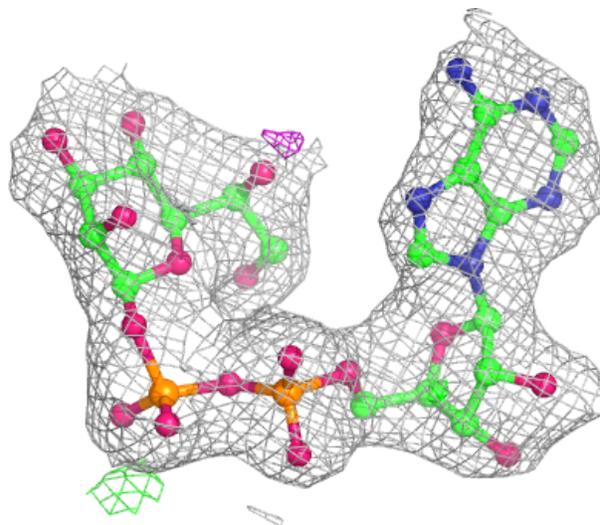
**Electron density around AYU I 501:**

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



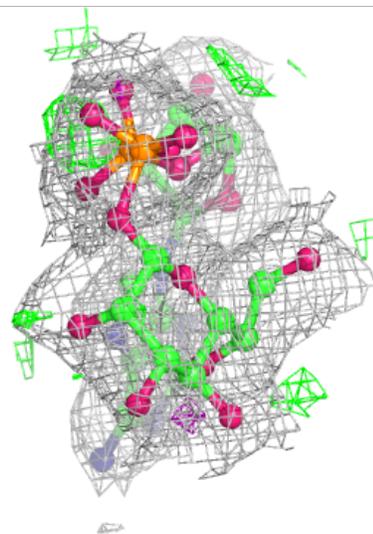
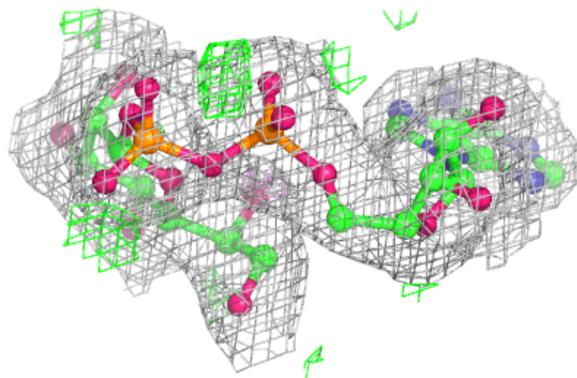
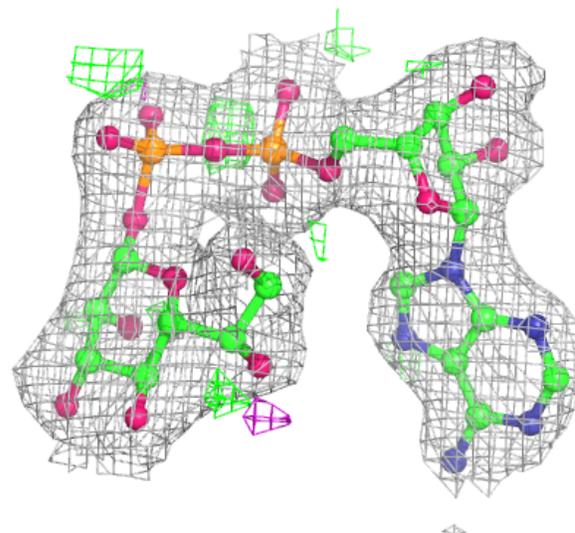
**Electron density around AYU F 501:**

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



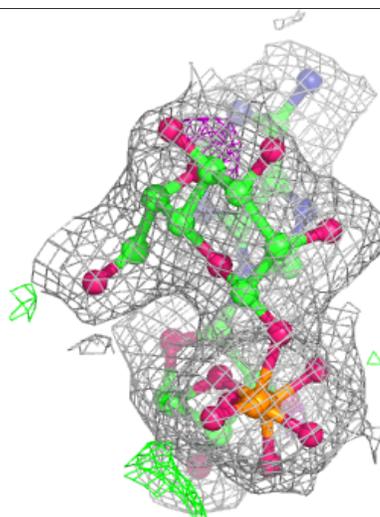
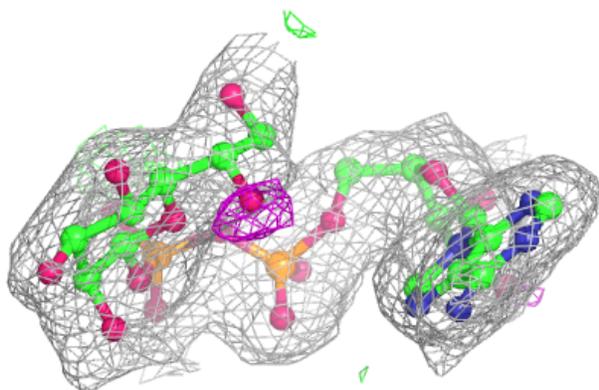
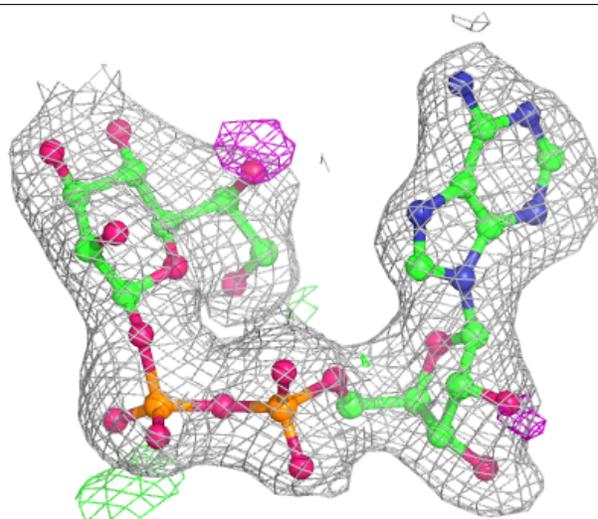
**Electron density around AYU A 501:**

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and green (positive)



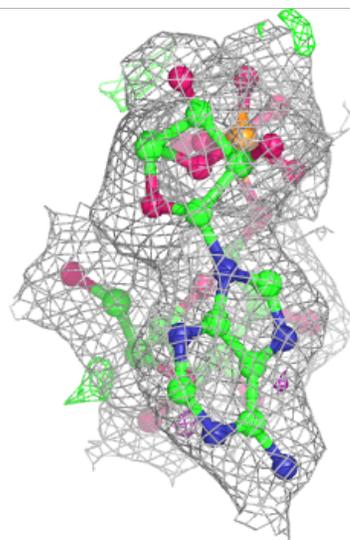
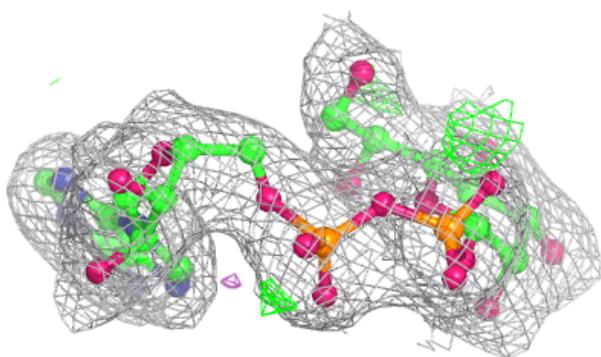
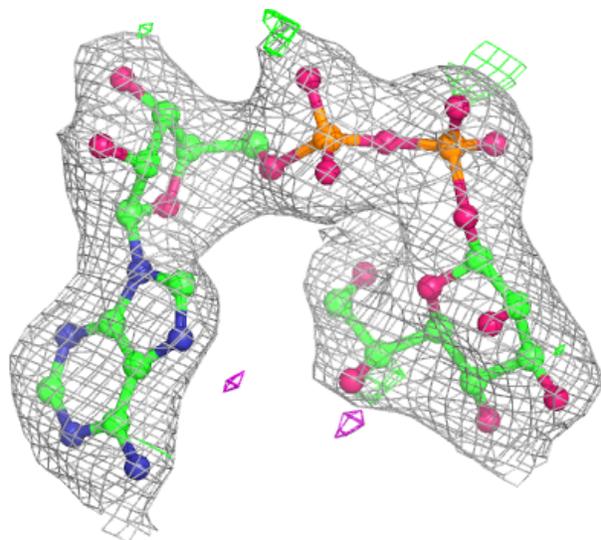
**Electron density around AYU D 501:**

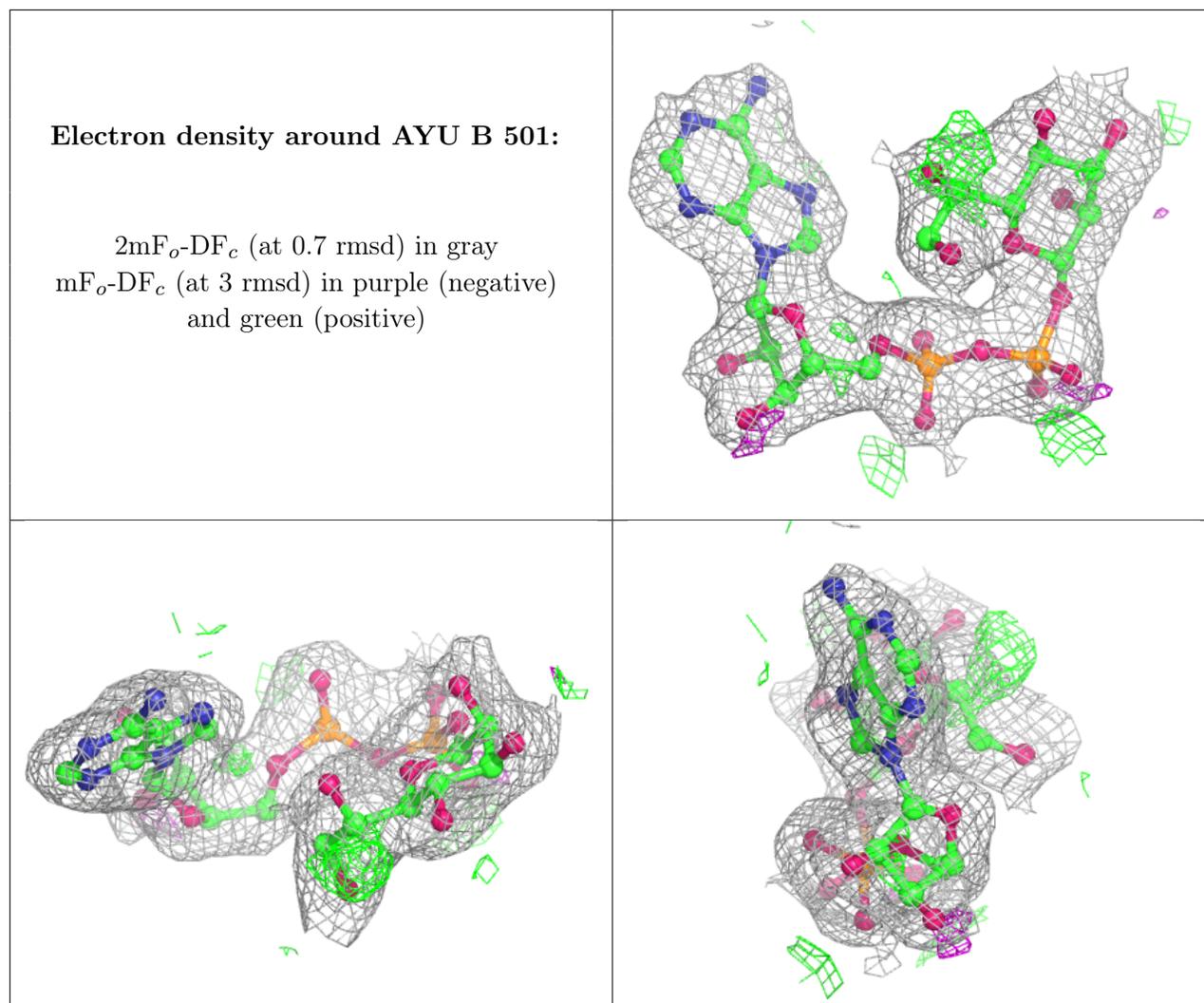
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around AYU E 501:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.