



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 08:37 am BST

PDB ID : 5C18  
Title : p97-delta709-728 in complex with ATP-gamma-S  
Authors : Haenzelmann, P.; Schindelin, H.  
Deposited on : 2015-06-13  
Resolution : 3.30 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 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 : 2.11  
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) : 2.11

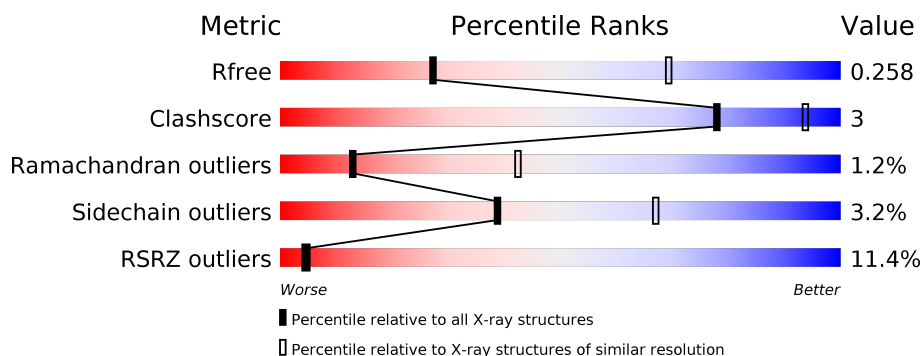
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 on 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	785	<div> <div>14%</div> <div>85%</div> <div>7% • 8%</div> </div>
1	B	785	<div> <div>5%</div> <div>82%</div> <div>9% • 8%</div> </div>
1	C	785	<div> <div>9%</div> <div>83%</div> <div>9% • 8%</div> </div>
1	D	785	<div> <div>14%</div> <div>84%</div> <div>7% • 8%</div> </div>
1	E	785	<div> <div>7%</div> <div>81%</div> <div>10% • 8%</div> </div>
1	F	785	<div> <div>14%</div> <div>83%</div> <div>8% • 8%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 69089 atoms, of which 34628 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	722	Total	C	H	N	O	S	0	0	0
			11409	3567	5741	1001	1070	30			
1	B	723	Total	C	H	N	O	S	0	0	0
			11420	3570	5746	1002	1072	30			
1	C	724	Total	C	H	N	O	S	0	0	0
			11427	3572	5749	1003	1073	30			
1	D	722	Total	C	H	N	O	S	0	0	0
			11409	3567	5741	1001	1070	30			
1	E	723	Total	C	H	N	O	S	0	0	0
			11418	3570	5745	1002	1071	30			
1	F	724	Total	C	H	N	O	S	0	0	0
			11430	3573	5750	1004	1073	30			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	ARG	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	ARG	deletion	UNP P55072
A	?	-	GLN	deletion	UNP P55072
A	?	-	THR	deletion	UNP P55072
A	?	-	ASN	deletion	UNP P55072
A	?	-	PRO	deletion	UNP P55072
A	?	-	SER	deletion	UNP P55072
A	?	-	ALA	deletion	UNP P55072
A	?	-	MET	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	VAL	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	GLU	deletion	UNP P55072
A	?	-	ASP	deletion	UNP P55072

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P55072
A	?	-	PRO	deletion	UNP P55072
A	?	-	VAL	deletion	UNP P55072
B	?	-	ARG	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	ARG	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	ARG	deletion	UNP P55072
B	?	-	GLN	deletion	UNP P55072
B	?	-	THR	deletion	UNP P55072
B	?	-	ASN	deletion	UNP P55072
B	?	-	PRO	deletion	UNP P55072
B	?	-	SER	deletion	UNP P55072
B	?	-	ALA	deletion	UNP P55072
B	?	-	MET	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	VAL	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	GLU	deletion	UNP P55072
B	?	-	ASP	deletion	UNP P55072
B	?	-	ASP	deletion	UNP P55072
B	?	-	PRO	deletion	UNP P55072
B	?	-	VAL	deletion	UNP P55072
C	?	-	ARG	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	ARG	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	ARG	deletion	UNP P55072
C	?	-	GLN	deletion	UNP P55072
C	?	-	THR	deletion	UNP P55072
C	?	-	ASN	deletion	UNP P55072
C	?	-	PRO	deletion	UNP P55072
C	?	-	SER	deletion	UNP P55072
C	?	-	ALA	deletion	UNP P55072
C	?	-	MET	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	VAL	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	GLU	deletion	UNP P55072
C	?	-	ASP	deletion	UNP P55072
C	?	-	ASP	deletion	UNP P55072
C	?	-	PRO	deletion	UNP P55072

*Continued on next page...*

*Continued from previous page...*

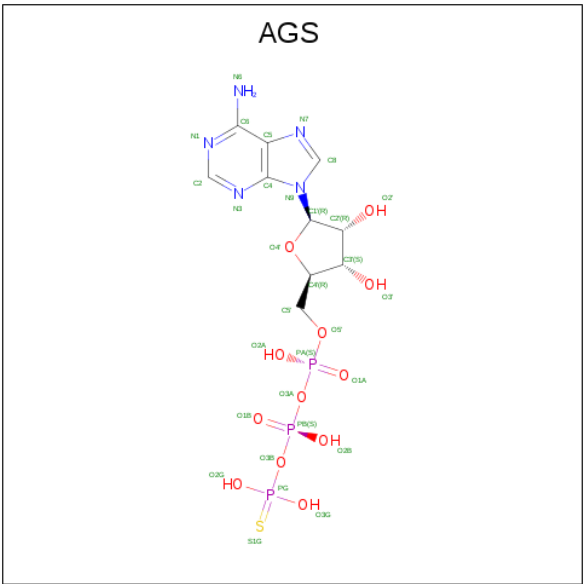
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	deletion	UNP P55072
D	?	-	ARG	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	ARG	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	ARG	deletion	UNP P55072
D	?	-	GLN	deletion	UNP P55072
D	?	-	THR	deletion	UNP P55072
D	?	-	ASN	deletion	UNP P55072
D	?	-	PRO	deletion	UNP P55072
D	?	-	SER	deletion	UNP P55072
D	?	-	ALA	deletion	UNP P55072
D	?	-	MET	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	VAL	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	GLU	deletion	UNP P55072
D	?	-	ASP	deletion	UNP P55072
D	?	-	ASP	deletion	UNP P55072
D	?	-	PRO	deletion	UNP P55072
D	?	-	VAL	deletion	UNP P55072
E	?	-	ARG	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	ARG	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	ARG	deletion	UNP P55072
E	?	-	GLN	deletion	UNP P55072
E	?	-	THR	deletion	UNP P55072
E	?	-	ASN	deletion	UNP P55072
E	?	-	PRO	deletion	UNP P55072
E	?	-	SER	deletion	UNP P55072
E	?	-	ALA	deletion	UNP P55072
E	?	-	MET	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	VAL	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	GLU	deletion	UNP P55072
E	?	-	ASP	deletion	UNP P55072
E	?	-	ASP	deletion	UNP P55072
E	?	-	PRO	deletion	UNP P55072
E	?	-	VAL	deletion	UNP P55072
F	?	-	ARG	deletion	UNP P55072

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLU	deletion	UNP P55072
F	?	-	ARG	deletion	UNP P55072
F	?	-	GLU	deletion	UNP P55072
F	?	-	ARG	deletion	UNP P55072
F	?	-	GLN	deletion	UNP P55072
F	?	-	THR	deletion	UNP P55072
F	?	-	ASN	deletion	UNP P55072
F	?	-	PRO	deletion	UNP P55072
F	?	-	SER	deletion	UNP P55072
F	?	-	ALA	deletion	UNP P55072
F	?	-	MET	deletion	UNP P55072
F	?	-	GLU	deletion	UNP P55072
F	?	-	VAL	deletion	UNP P55072
F	?	-	GLU	deletion	UNP P55072
F	?	-	GLU	deletion	UNP P55072
F	?	-	ASP	deletion	UNP P55072
F	?	-	ASP	deletion	UNP P55072
F	?	-	PRO	deletion	UNP P55072
F	?	-	VAL	deletion	UNP P55072

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		
3	F	2	Total	Mg	0	0
			2	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

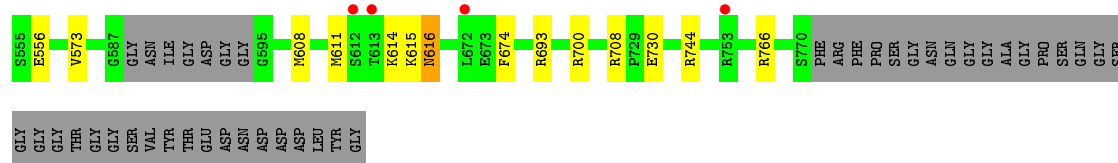
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

- Molecule 5 is water.

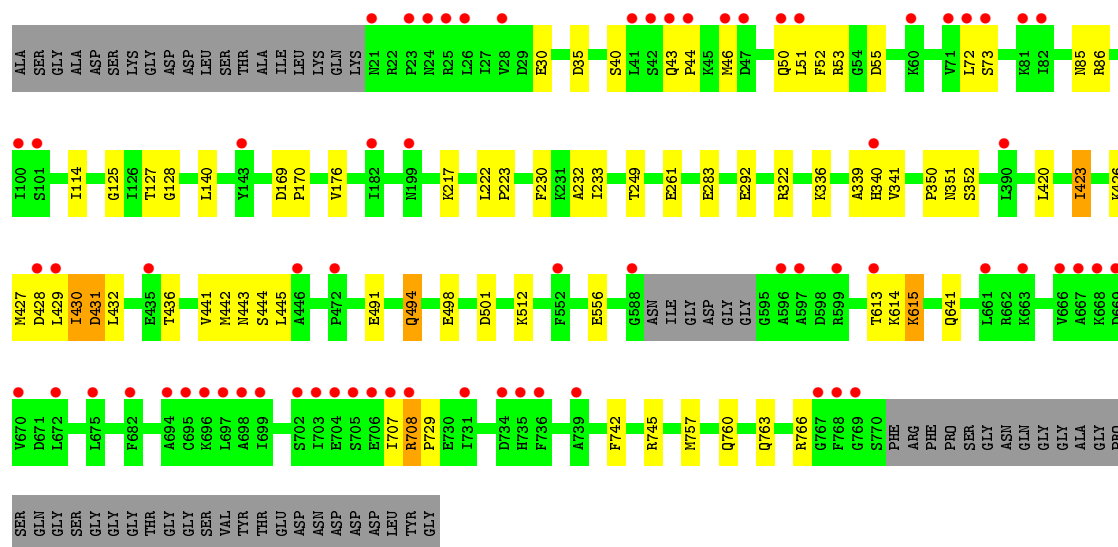
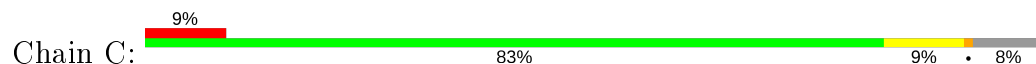
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	B	5	Total O 5 5	0	0
5	C	5	Total O 5 5	0	0
5	D	5	Total O 5 5	0	0
5	E	5	Total O 5 5	0	0
5	F	5	Total O 5 5	0	0



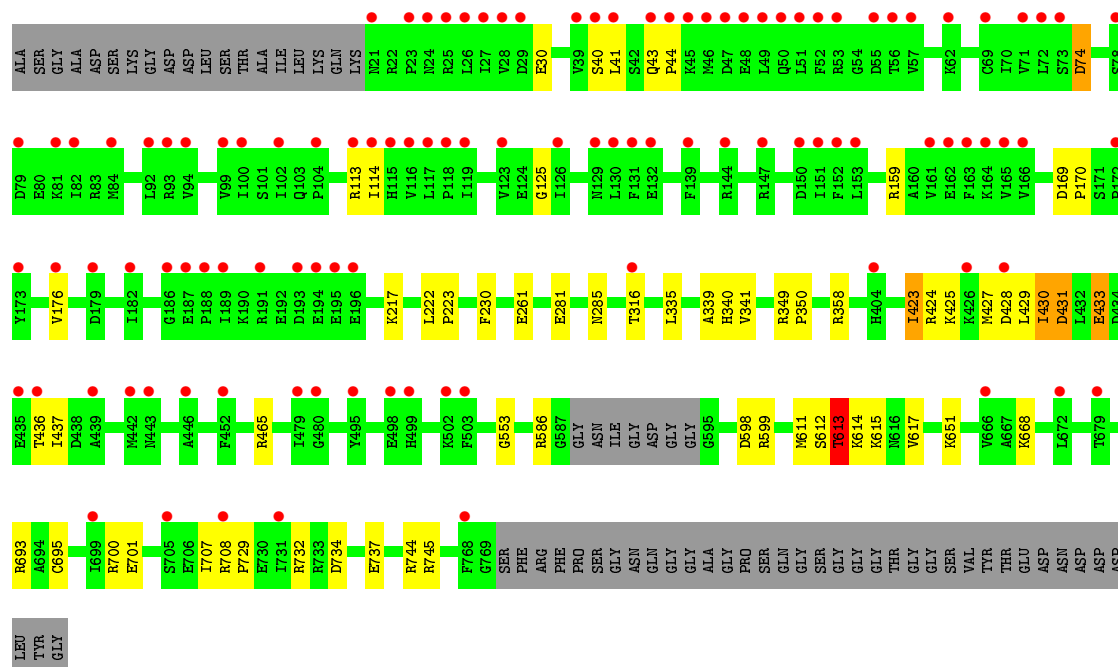
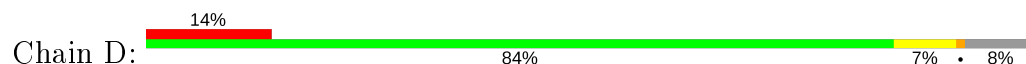




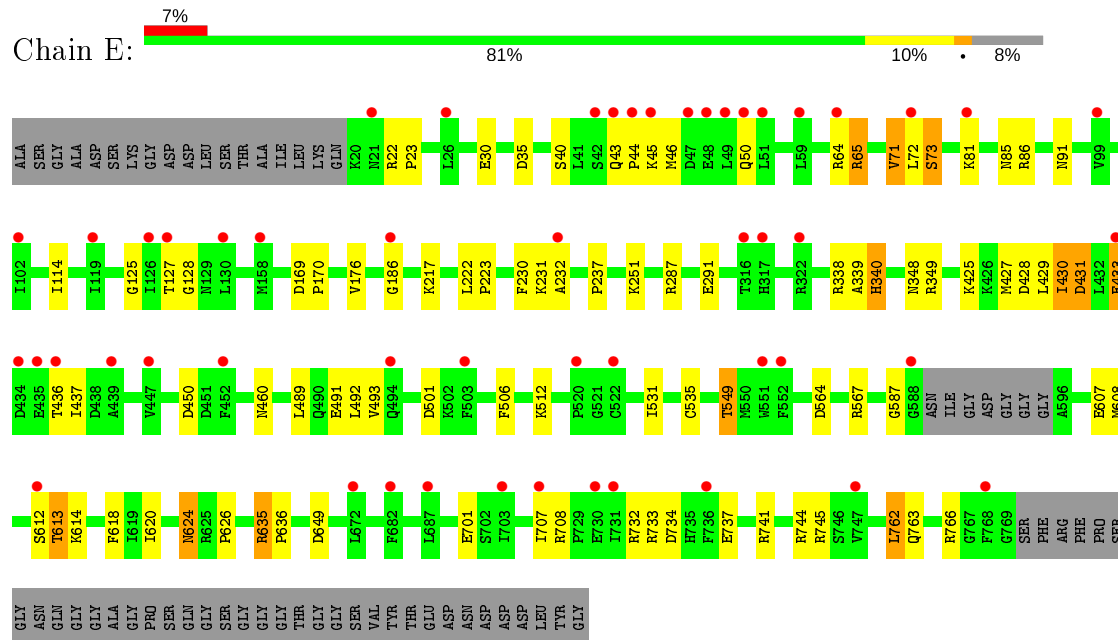
• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.33Å 180.06Å 255.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.30 49.18 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-3.30) 100.0 (49.18-3.30)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.211 , 0.249 0.222 , 0.258	Depositor DCC
$R_{free}$ test set	4893 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	101.3	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 77.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	69089	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: MG, AGS, CL

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	0.22	0/5761	0.40	0/7778
1	B	0.22	0/5767	0.41	0/7786
1	C	0.23	0/5771	0.41	0/7791
1	D	0.22	0/5761	0.40	0/7778
1	E	0.22	0/5766	0.41	0/7785
1	F	0.22	0/5773	0.40	0/7794
All	All	0.22	0/34599	0.40	0/46712

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	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	339	ALA	Peptide

### 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	5668	5741	5741	30	0
1	B	5674	5746	5746	39	0
1	C	5678	5749	5749	34	0
1	D	5668	5741	5741	32	0
1	E	5673	5745	5743	45	0
1	F	5680	5750	5750	32	0
2	A	62	26	24	2	0
2	B	62	26	24	3	0
2	C	62	26	24	0	0
2	D	62	26	24	0	0
2	E	62	26	24	2	0
2	F	62	26	24	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	2	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	1	0
5	F	5	0	0	1	0
All	All	34461	34628	34614	201	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 3.

The worst 5 of 201 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:B:512:LYS:NZ	1:B:608:MET:O	2.14	0.81
1:F:313:ARG:NH2	1:F:326:SER:OG	2.18	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:512:LYS:NZ	1:F:608:MET:O	2.20	0.75
1:A:653:ARG:NH2	1:A:676:ALA:O	2.20	0.75
1:A:65:ARG:NH1	1:A:91:ASN:O	2.19	0.75

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	718/785 (92%)	682 (95%)	31 (4%)	5 (1%)	22	54
1	B	719/785 (92%)	667 (93%)	44 (6%)	8 (1%)	14	45
1	C	720/785 (92%)	673 (94%)	35 (5%)	12 (2%)	9	35
1	D	718/785 (92%)	673 (94%)	37 (5%)	8 (1%)	14	45
1	E	719/785 (92%)	668 (93%)	41 (6%)	10 (1%)	11	38
1	F	720/785 (92%)	668 (93%)	44 (6%)	8 (1%)	14	45
All	All	4314/4710 (92%)	4031 (93%)	232 (5%)	51 (1%)	13	42

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	80	GLU
1	B	428	ASP
1	B	615	LYS
1	C	50	GLN
1	C	352	SER

### 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	616/658 (94%)	600 (97%)	16 (3%)	46	71
1	B	617/658 (94%)	591 (96%)	26 (4%)	30	60
1	C	617/658 (94%)	596 (97%)	21 (3%)	37	65
1	D	616/658 (94%)	600 (97%)	16 (3%)	46	71
1	E	616/658 (94%)	590 (96%)	26 (4%)	30	60
1	F	617/658 (94%)	602 (98%)	15 (2%)	49	73
All	All	3699/3948 (94%)	3579 (97%)	120 (3%)	39	67

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	442	MET
1	D	261	GLU
1	F	433	GLU
1	C	443	ASN
1	C	742	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	348	ASN
1	B	616	ASN
1	D	21	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 18 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
2	AGS	A	901	3	26,33,33	1.56	8 (30%)	26,52,52	1.84	6 (23%)
2	AGS	E	901	3	26,33,33	1.54	8 (30%)	26,52,52	1.82	5 (19%)
2	AGS	B	901	3	26,33,33	1.58	8 (30%)	26,52,52	1.64	5 (19%)
2	AGS	D	901	3	26,33,33	1.53	8 (30%)	26,52,52	1.76	6 (23%)
2	AGS	F	901	3	26,33,33	1.55	7 (26%)	26,52,52	1.67	3 (11%)
2	AGS	D	902	3	26,33,33	1.59	8 (30%)	26,52,52	1.68	5 (19%)
2	AGS	C	902	3	26,33,33	1.58	8 (30%)	26,52,52	1.67	3 (11%)
2	AGS	B	902	3	26,33,33	1.62	8 (30%)	26,52,52	1.54	4 (15%)
2	AGS	A	902	3	26,33,33	1.59	8 (30%)	26,52,52	1.53	3 (11%)
2	AGS	C	901	3	26,33,33	1.55	8 (30%)	26,52,52	1.76	5 (19%)
2	AGS	F	902	3	26,33,33	1.58	8 (30%)	26,52,52	1.61	4 (15%)
2	AGS	E	902	3	26,33,33	1.58	7 (26%)	26,52,52	1.60	4 (15%)

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	AGS	A	901	3	-	3/17/38/38	0/3/3/3
2	AGS	E	901	3	-	7/17/38/38	0/3/3/3
2	AGS	B	901	3	-	5/17/38/38	0/3/3/3
2	AGS	D	901	3	-	10/17/38/38	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AGS	F	901	3	-	2/17/38/38	0/3/3/3
2	AGS	D	902	3	-	2/17/38/38	0/3/3/3
2	AGS	C	902	3	-	3/17/38/38	0/3/3/3
2	AGS	B	902	3	-	7/17/38/38	0/3/3/3
2	AGS	A	902	3	-	3/17/38/38	0/3/3/3
2	AGS	C	901	3	-	10/17/38/38	0/3/3/3
2	AGS	F	902	3	-	4/17/38/38	0/3/3/3
2	AGS	E	902	3	-	2/17/38/38	0/3/3/3

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	AGS	C2'-C1'	-3.71	1.48	1.53
2	B	902	AGS	C2'-C1'	-3.63	1.48	1.53
2	D	902	AGS	C2'-C1'	-3.62	1.48	1.53
2	F	902	AGS	C2'-C1'	-3.51	1.48	1.53
2	E	902	AGS	C2'-C1'	-3.51	1.48	1.53

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	901	AGS	N3-C2-N1	-5.59	119.94	128.68
2	C	902	AGS	N3-C2-N1	-5.56	120.00	128.68
2	E	901	AGS	N3-C2-N1	-5.55	120.00	128.68
2	D	902	AGS	N3-C2-N1	-5.54	120.01	128.68
2	A	901	AGS	N3-C2-N1	-5.52	120.06	128.68

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

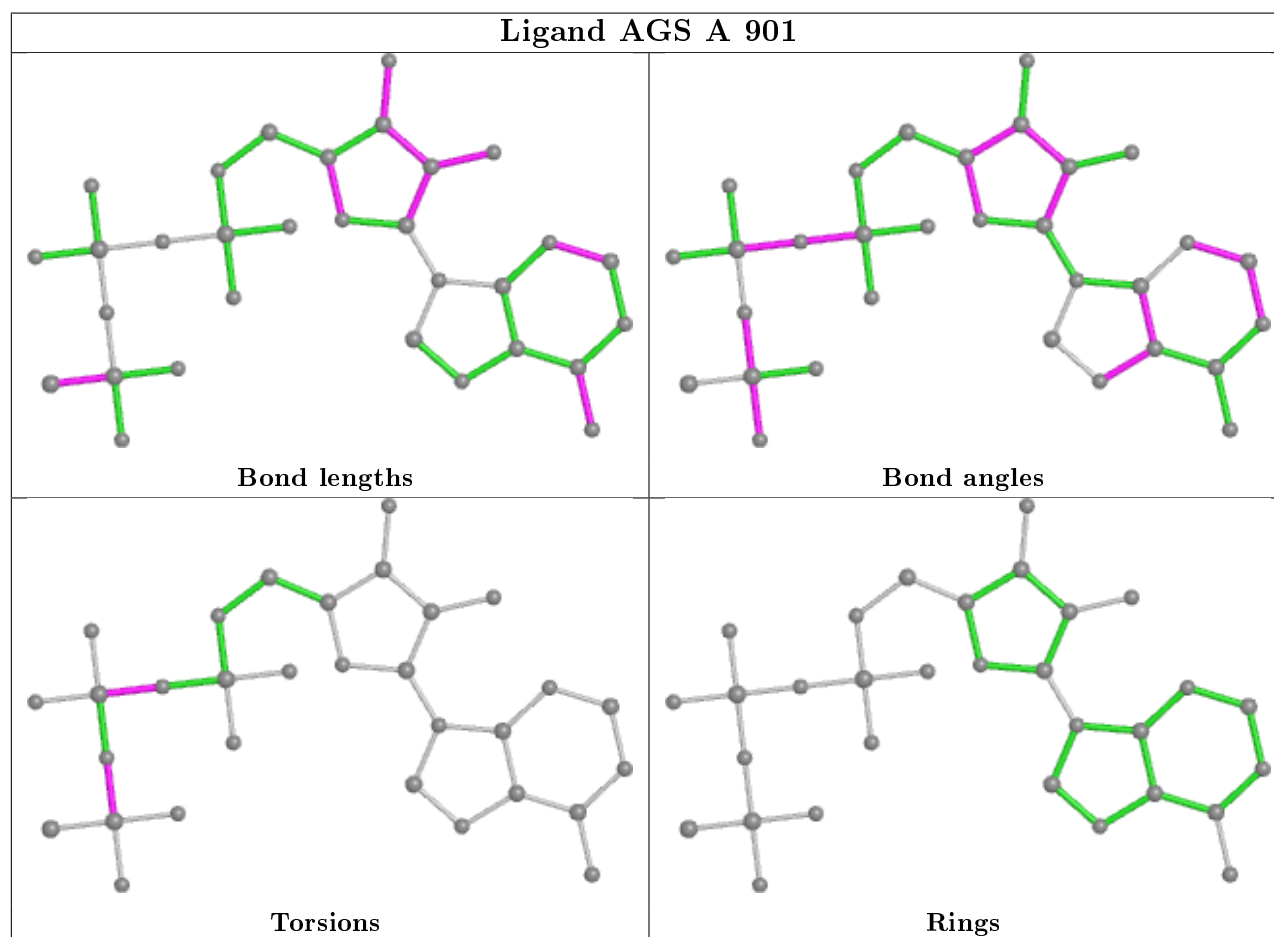
Mol	Chain	Res	Type	Atoms
2	E	901	AGS	PB-O3B-PG-O2G
2	E	901	AGS	PB-O3B-PG-O3G
2	E	901	AGS	C5'-O5'-PA-O2A
2	E	901	AGS	C5'-O5'-PA-O3A
2	E	901	AGS	O4'-C4'-C5'-O5'

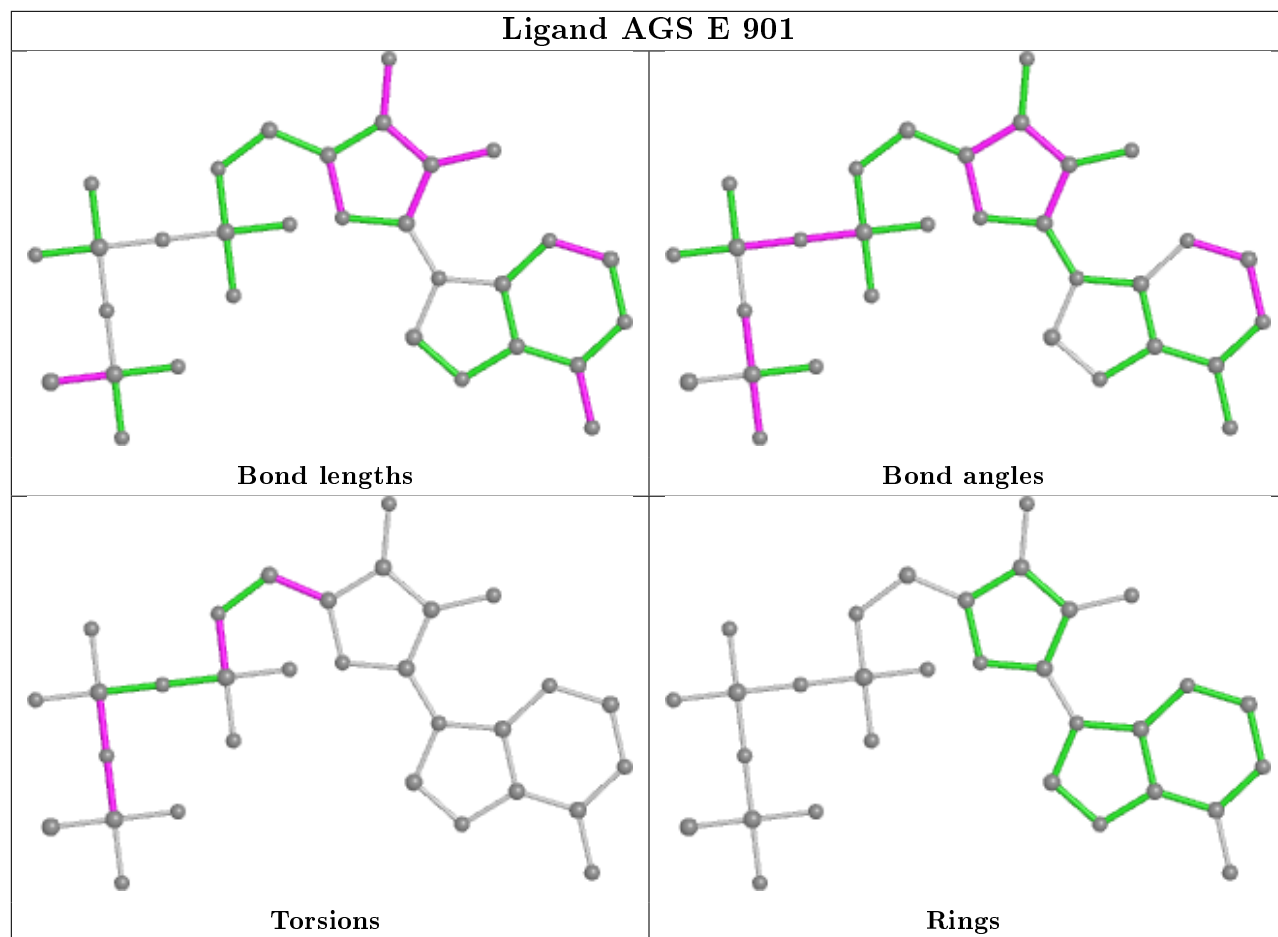
There are no ring outliers.

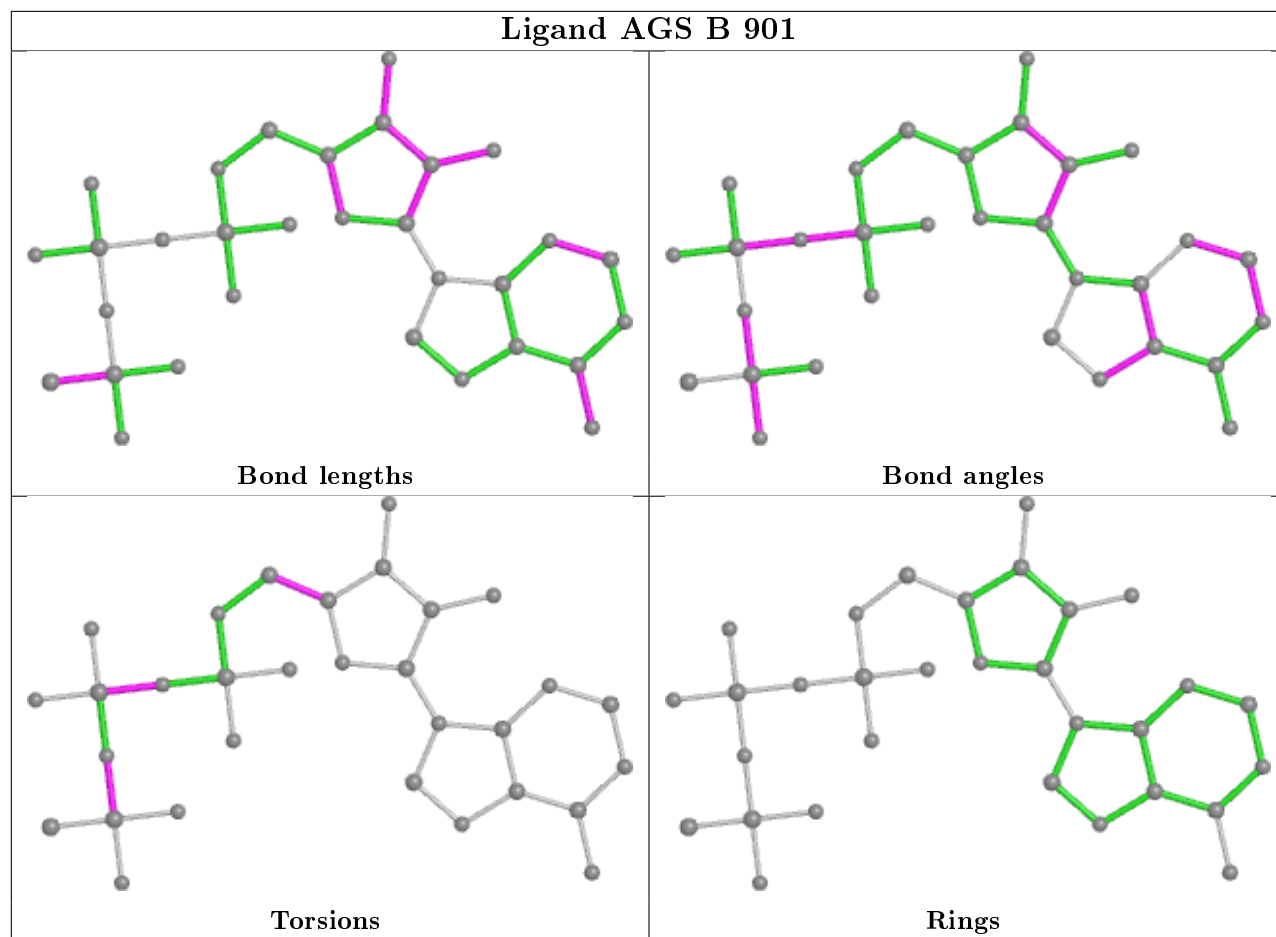
6 monomers are involved in 9 short contacts:

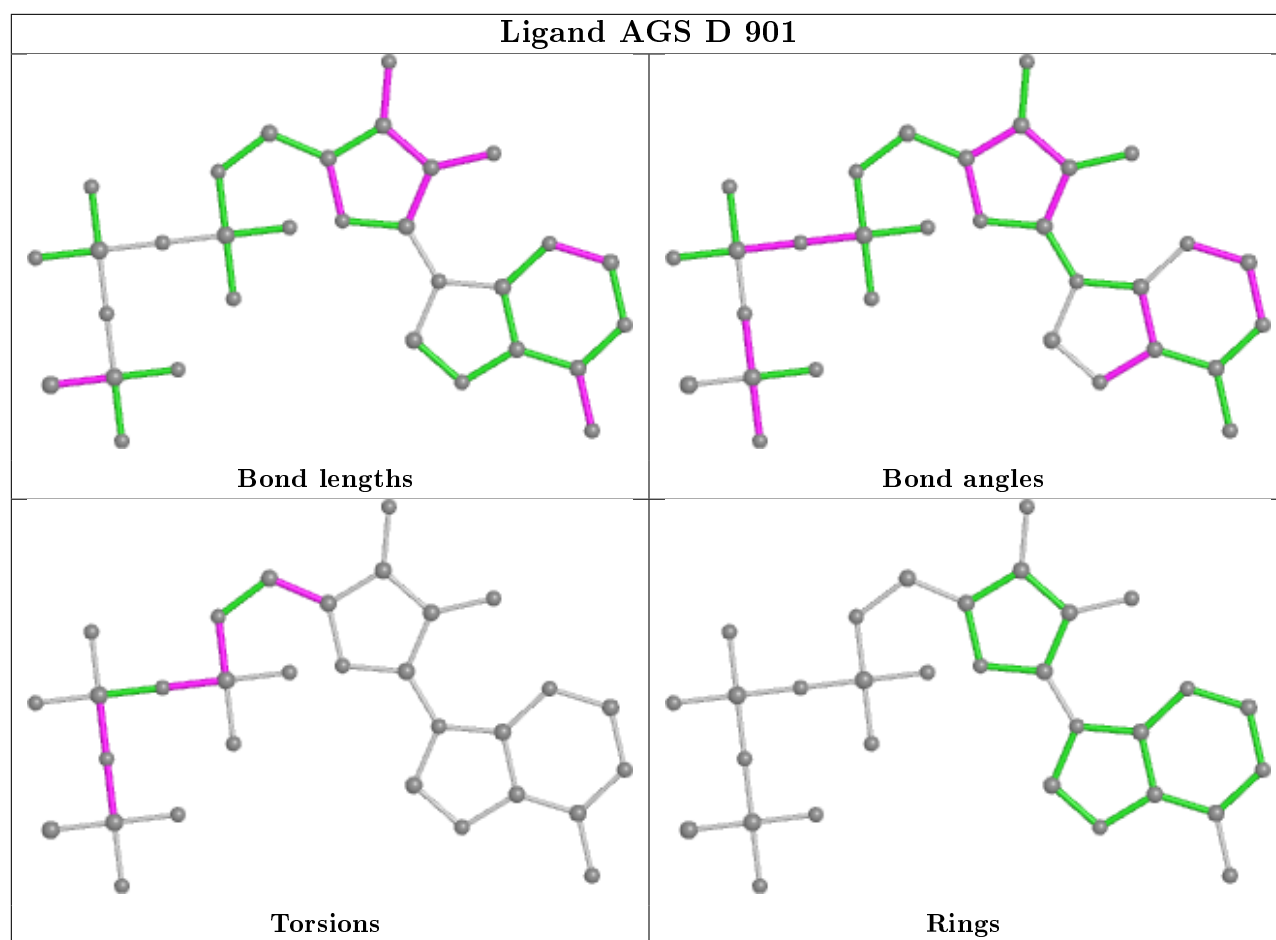
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	AGS	1	0
2	B	901	AGS	2	0
2	B	902	AGS	1	0
2	A	902	AGS	1	0
2	F	902	AGS	2	0
2	E	902	AGS	2	0

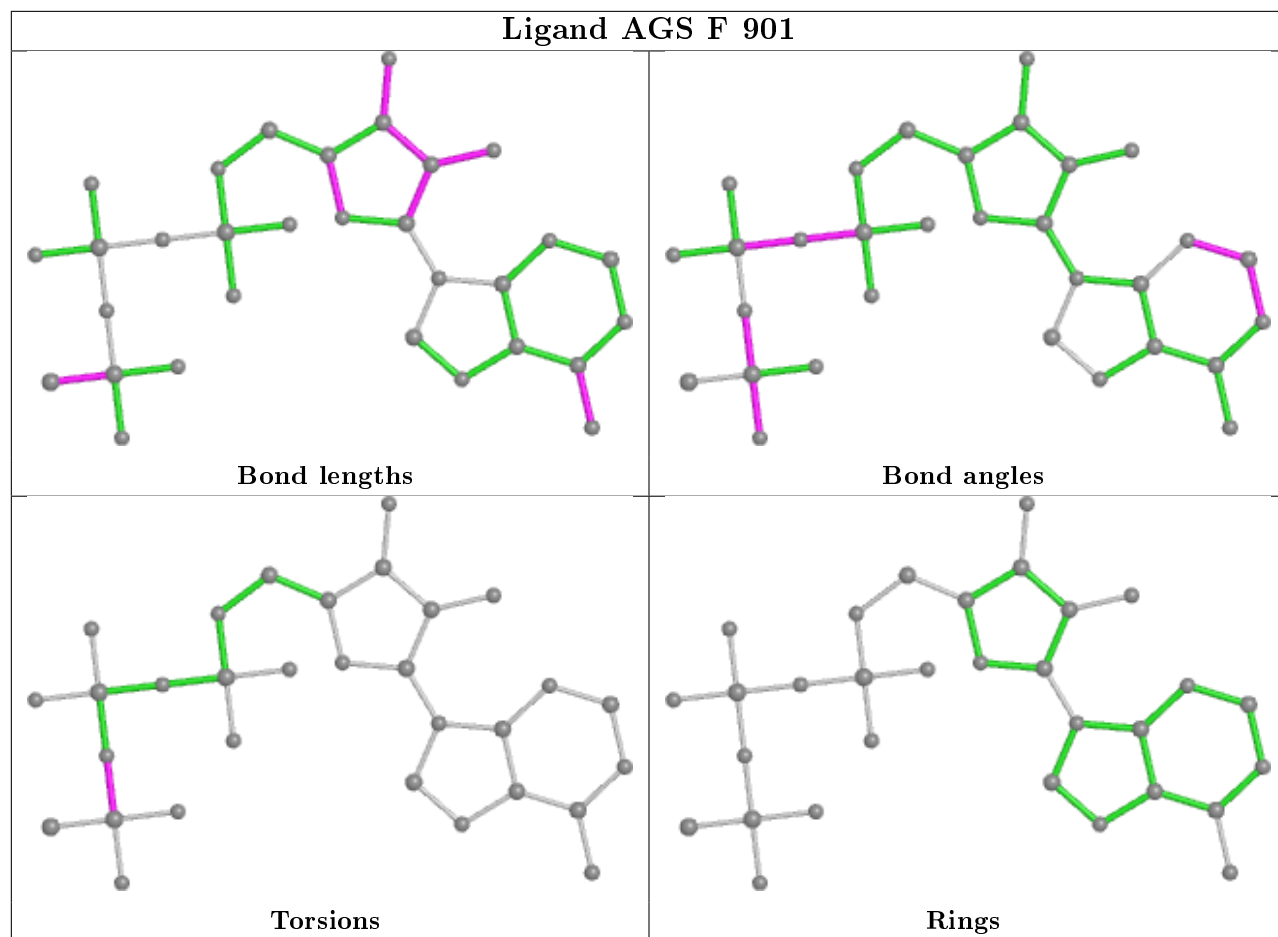
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

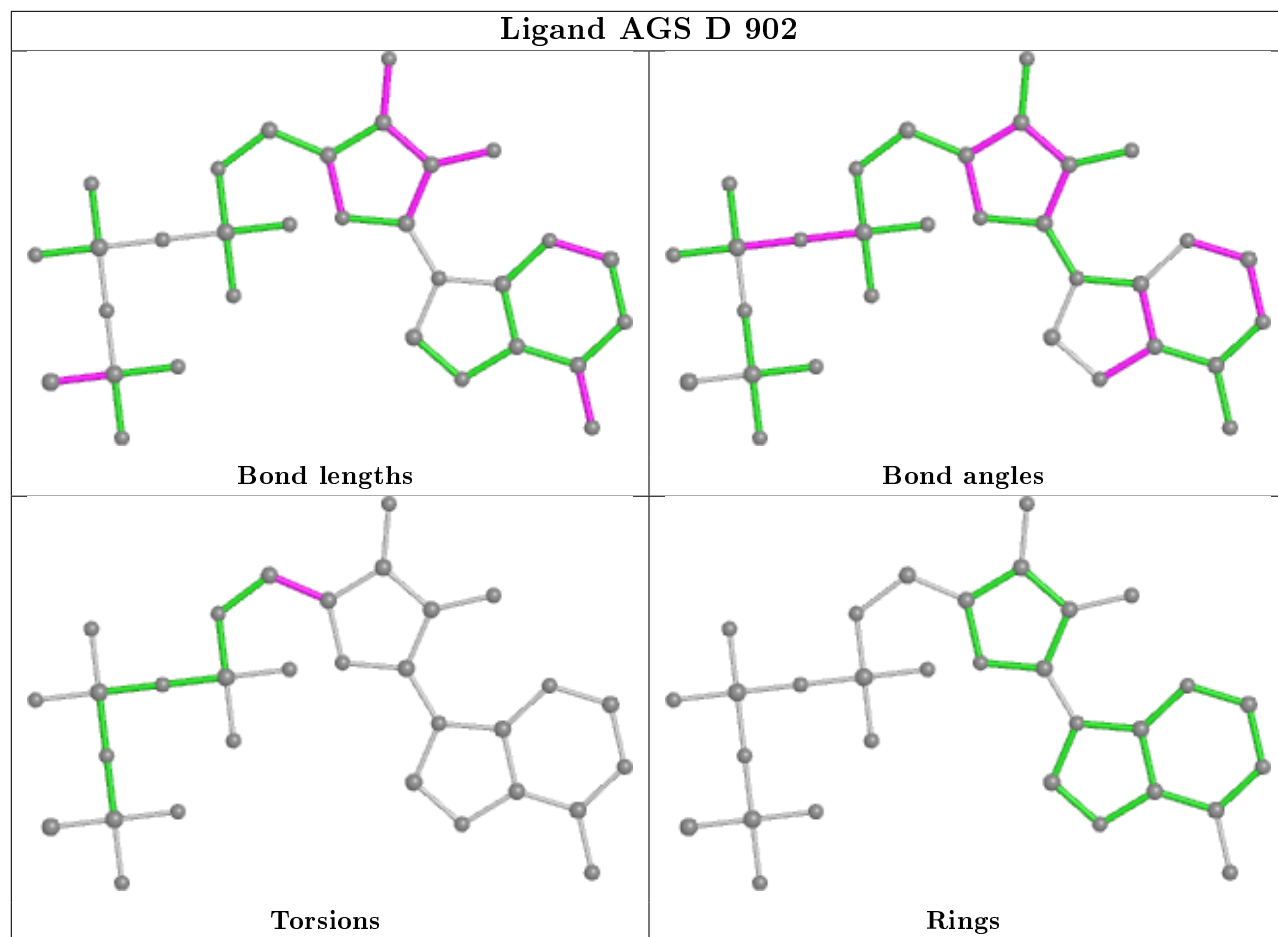




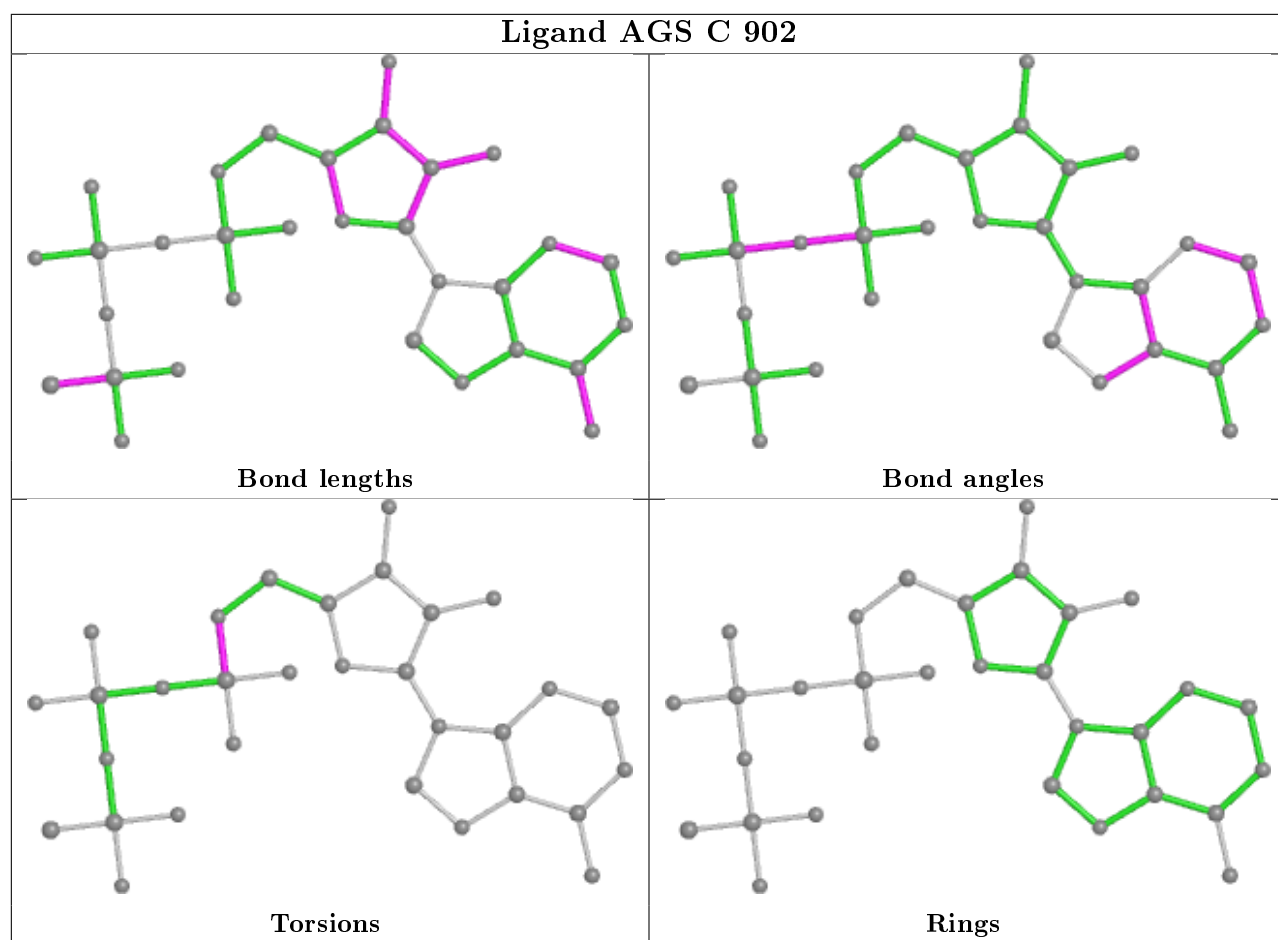


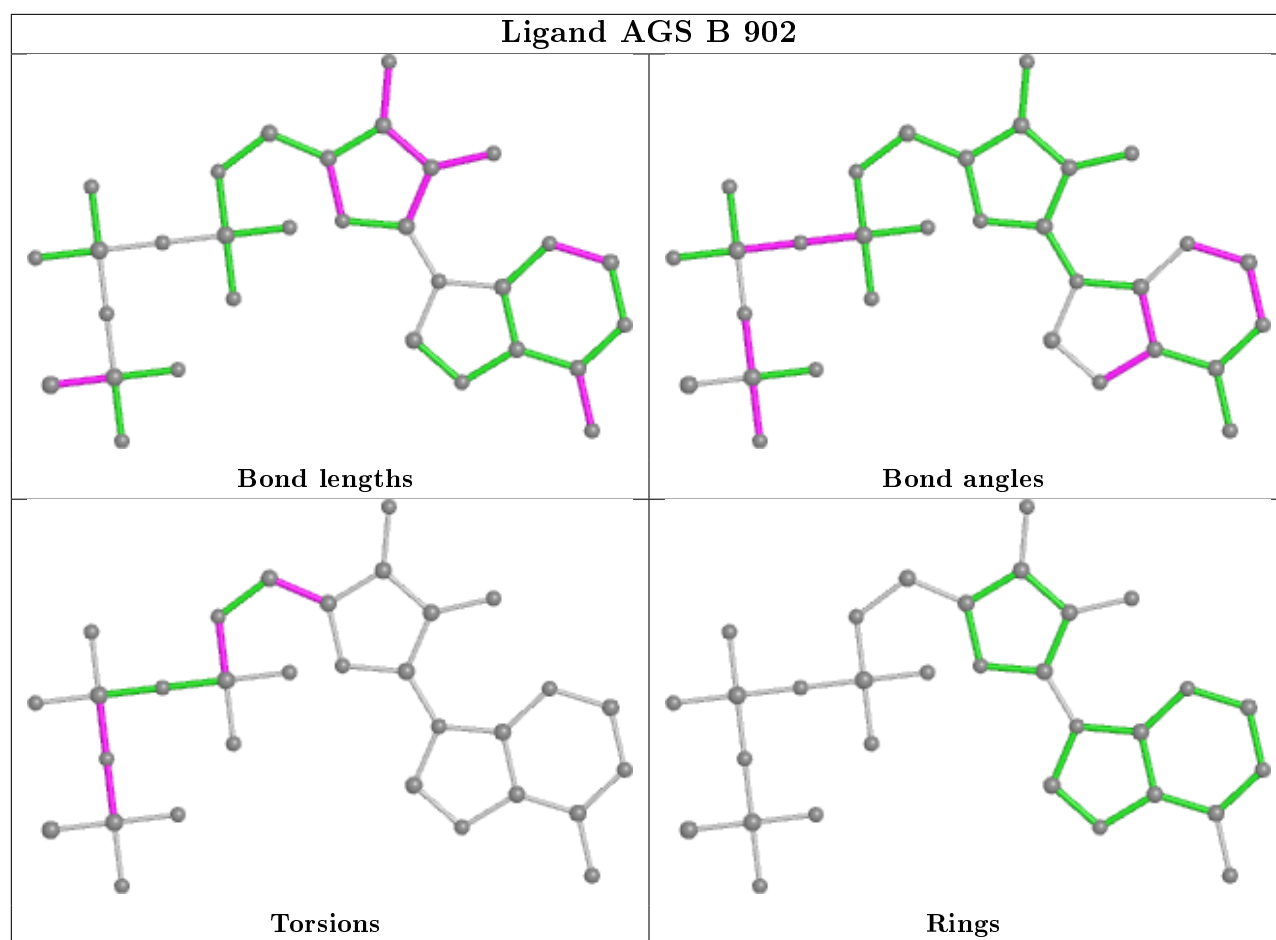


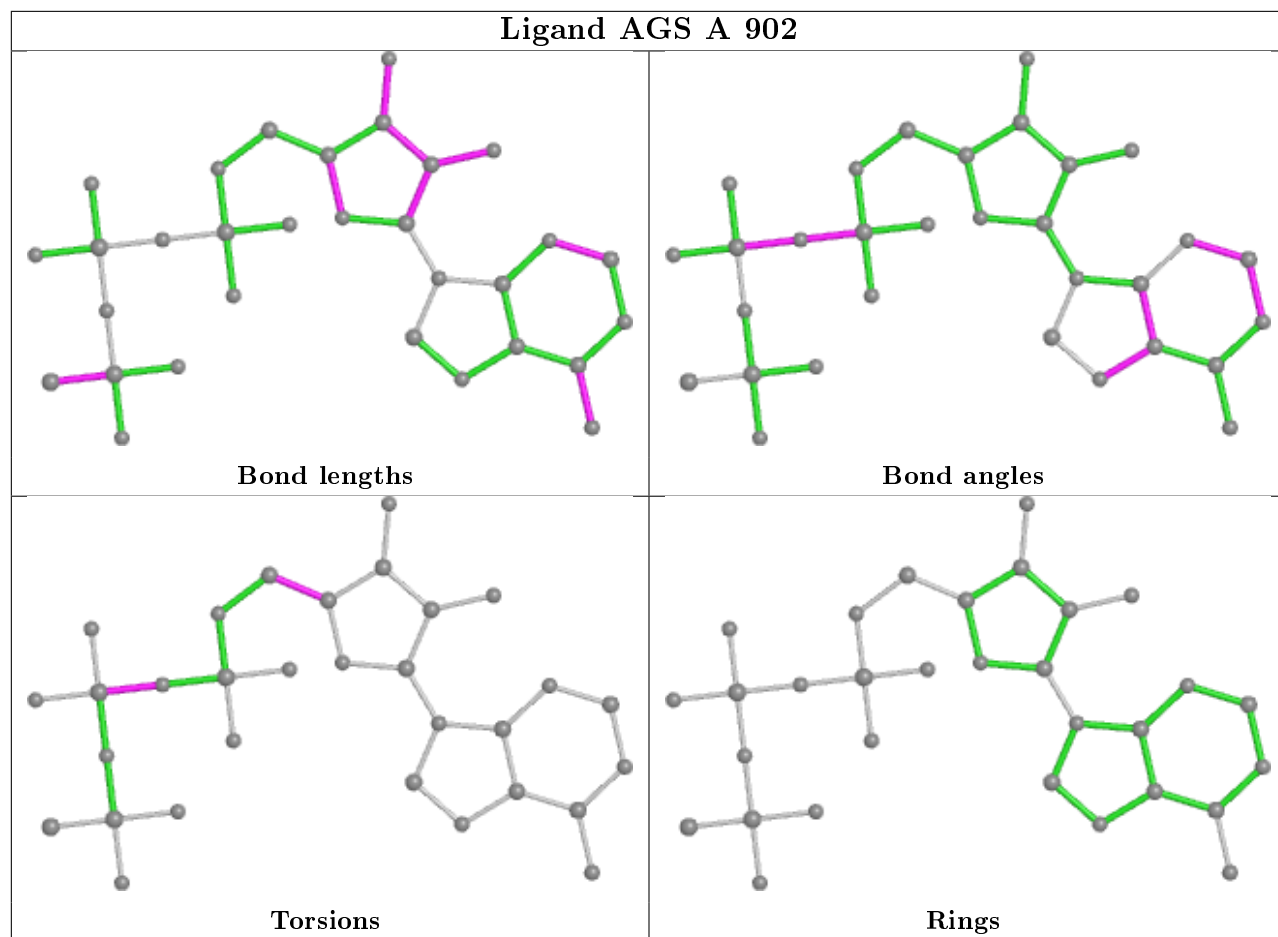


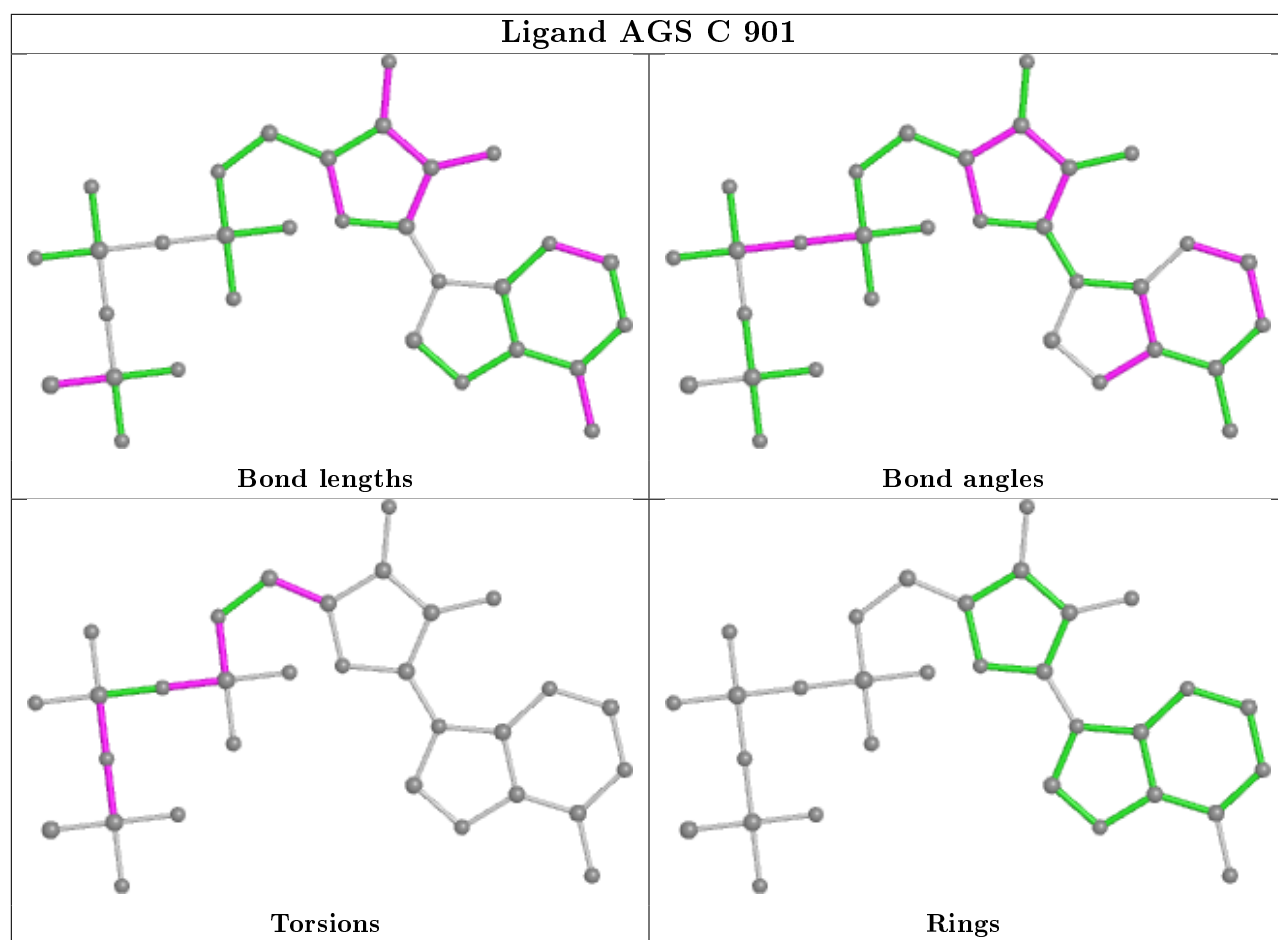


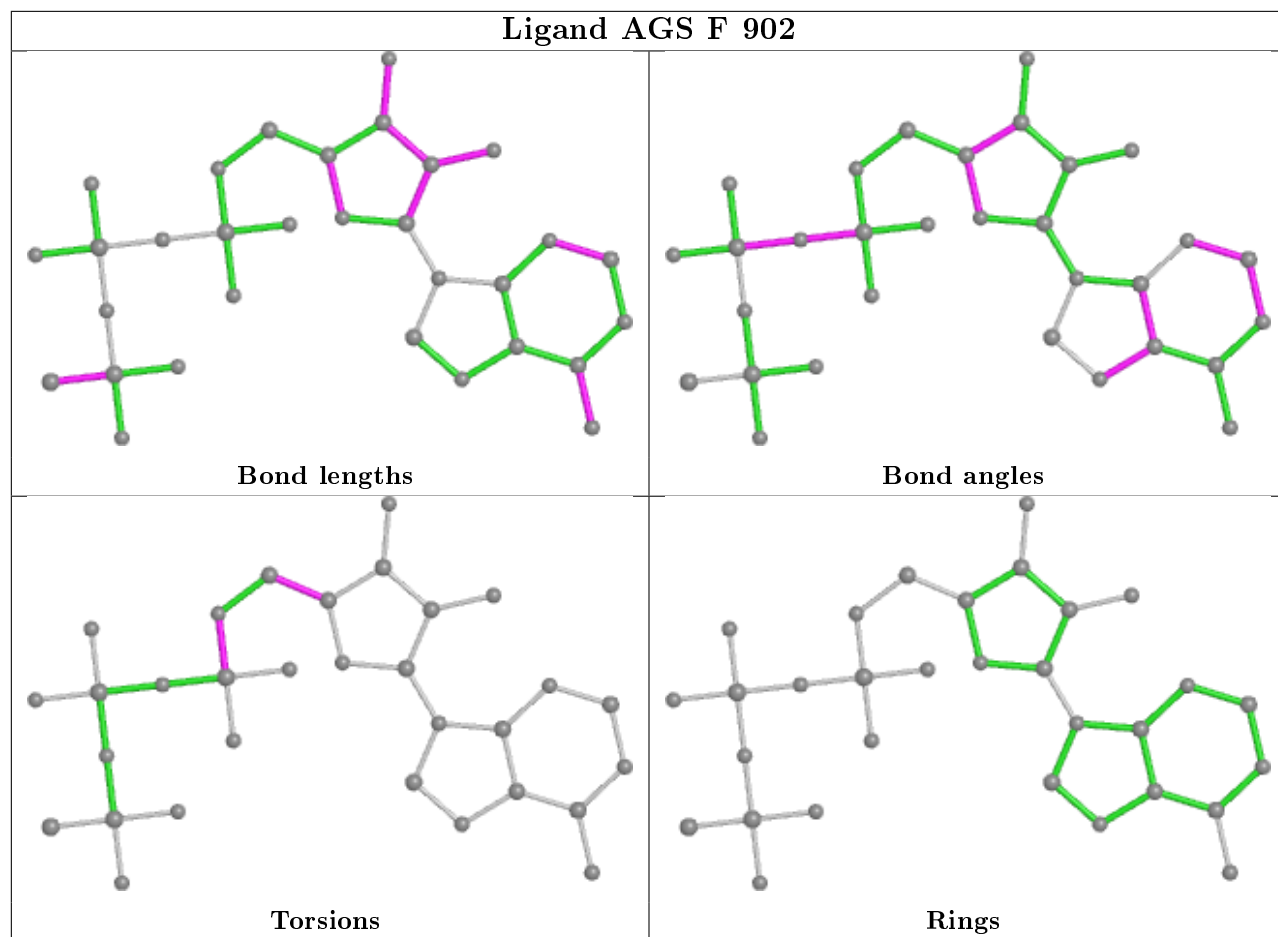


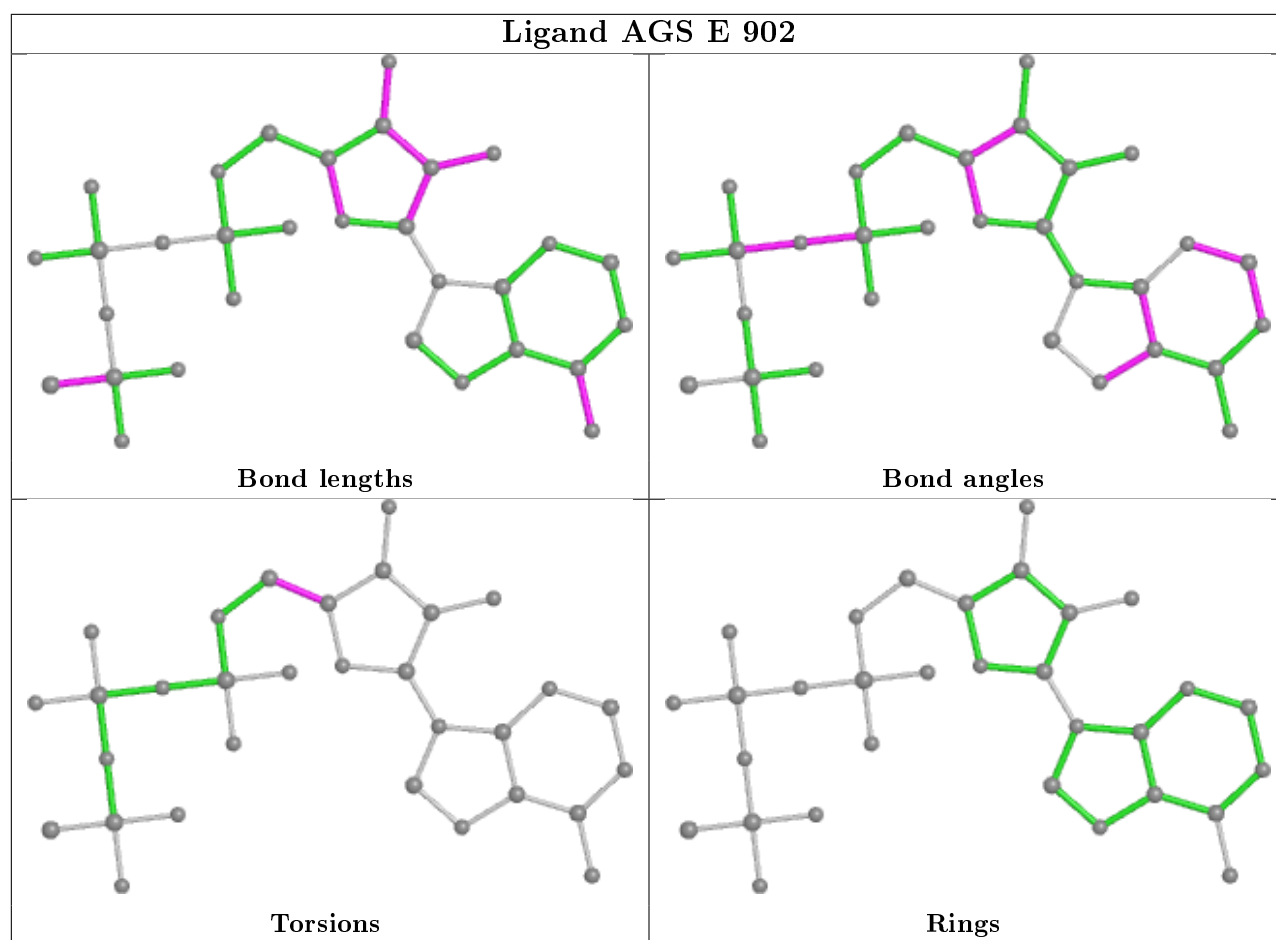












## 5.7 Other polymers [i](#)

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	722/785 (91%)	0.94	112 (15%) <b>2</b> <b>2</b>	53, 121, 220, 294	0
1	B	723/785 (92%)	0.55	40 (5%) <b>25</b> <b>23</b>	53, 108, 176, 299	0
1	C	724/785 (92%)	0.60	69 (9%) <b>8</b> <b>8</b>	42, 113, 191, 278	0
1	D	722/785 (91%)	0.83	108 (14%) <b>2</b> <b>2</b>	53, 135, 220, 266	0
1	E	723/785 (92%)	0.59	52 (7%) <b>15</b> <b>15</b>	63, 113, 181, 272	0
1	F	724/785 (92%)	0.93	113 (15%) <b>2</b> <b>2</b>	47, 122, 233, 304	0
All	All	4338/4710 (92%)	0.74	494 (11%) <b>5</b> <b>4</b>	42, 117, 213, 304	0

The worst 5 of 494 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	116	VAL	11.9
1	F	24	ASN	9.8
1	F	114	ILE	8.9
1	F	102	ILE	7.5
1	D	46	MET	7.4

### 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 carbohydrates 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.

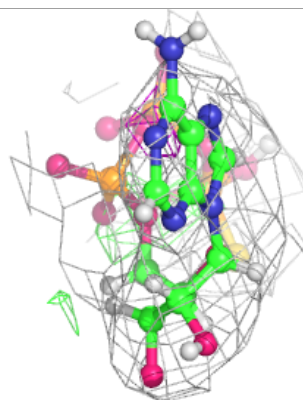
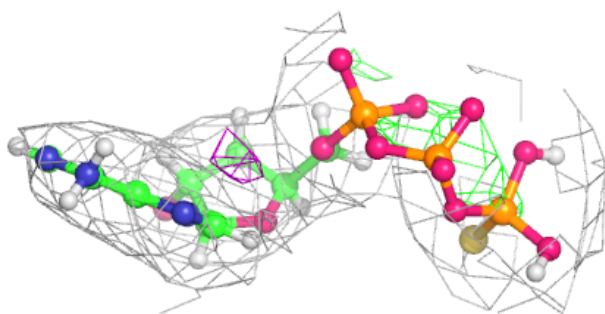
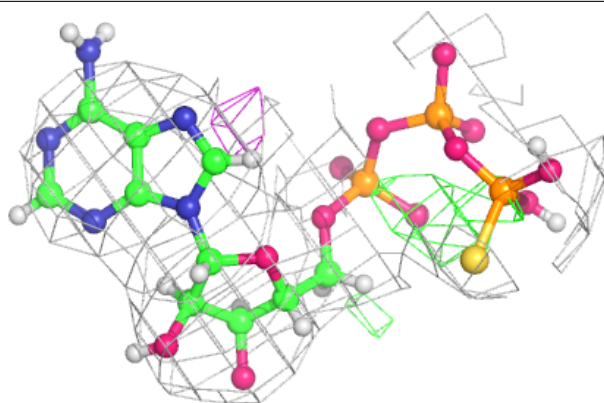
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	D	903	1/1	0.84	0.13	170,170,170,170	0
4	CL	F	905	1/1	0.86	0.31	98,98,98,98	0
4	CL	C	905	1/1	0.86	0.20	117,117,117,117	0
4	CL	D	905	1/1	0.87	0.24	99,99,99,99	0
4	CL	B	905	1/1	0.88	0.23	92,92,92,92	0
4	CL	E	905	1/1	0.89	0.28	93,93,93,93	0
2	AGS	E	901	31/31	0.91	0.26	76,88,120,170	0
4	CL	A	905	1/1	0.91	0.28	87,87,87,87	0
3	MG	A	903	1/1	0.94	0.12	186,186,186,186	0
2	AGS	B	901	31/31	0.94	0.24	57,88,112,122	0
2	AGS	D	901	31/31	0.94	0.24	70,99,121,158	0
2	AGS	C	901	31/31	0.94	0.20	59,100,122,152	0
2	AGS	A	901	31/31	0.95	0.27	75,86,104,117	0
2	AGS	D	902	31/31	0.95	0.21	68,82,106,169	0
2	AGS	F	901	31/31	0.95	0.24	47,61,80,93	0
2	AGS	F	902	31/31	0.95	0.24	88,102,133,210	0
3	MG	F	904	1/1	0.96	0.27	76,76,76,76	0
2	AGS	E	902	31/31	0.96	0.20	75,89,127,165	0
3	MG	F	903	1/1	0.96	0.16	152,152,152,152	0
3	MG	D	904	1/1	0.96	0.31	99,99,99,99	0
2	AGS	C	902	31/31	0.96	0.26	59,76,122,189	0
3	MG	A	904	1/1	0.97	0.23	76,76,76,76	0
2	AGS	B	902	31/31	0.97	0.23	55,79,132,182	0
2	AGS	A	902	31/31	0.97	0.26	73,90,154,194	0
3	MG	E	903	1/1	0.97	0.14	81,81,81,81	0
3	MG	C	904	1/1	0.98	0.22	107,107,107,107	0
3	MG	B	903	1/1	0.98	0.17	119,119,119,119	0
3	MG	C	903	1/1	0.98	0.23	101,101,101,101	0
3	MG	E	904	1/1	0.98	0.26	96,96,96,96	0
3	MG	B	904	1/1	0.98	0.22	86,86,86,86	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.

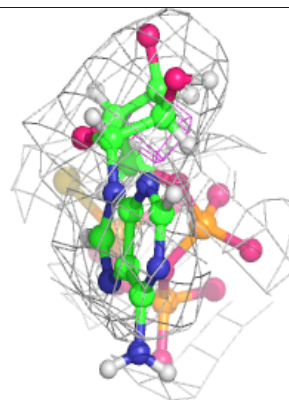
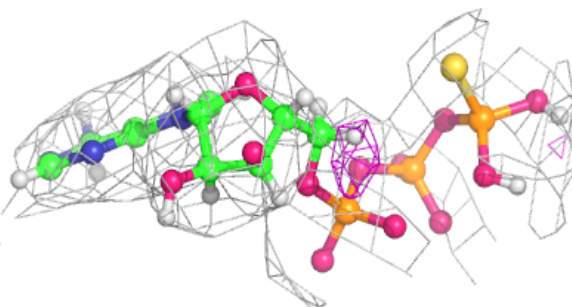
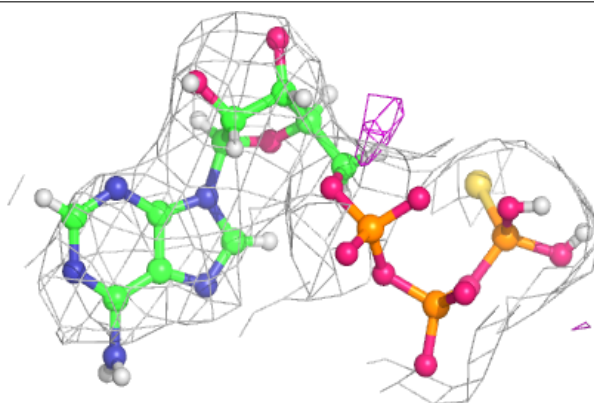


**Electron density around AGS E 901:**

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

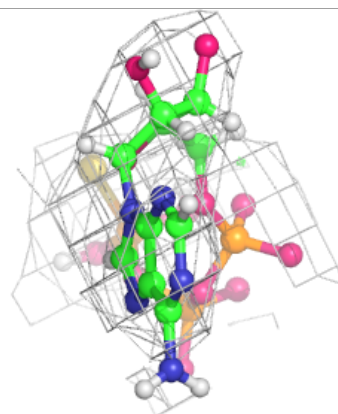
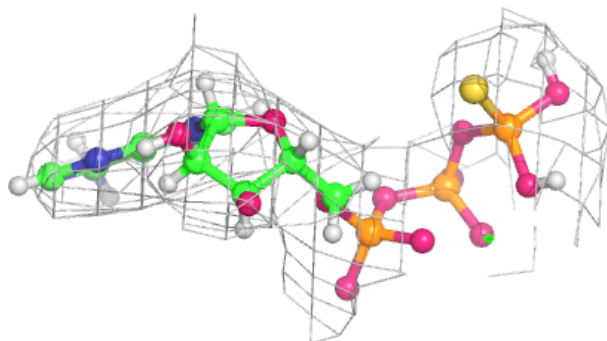
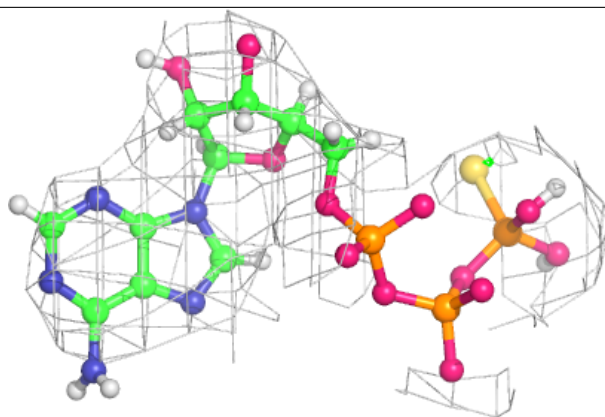
**Electron density around AGS B 901:**

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

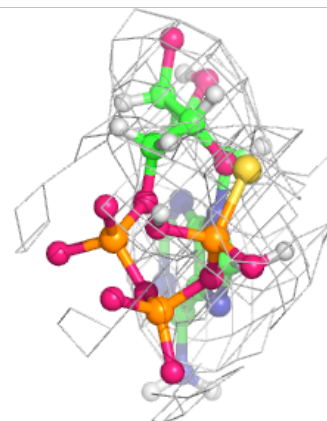
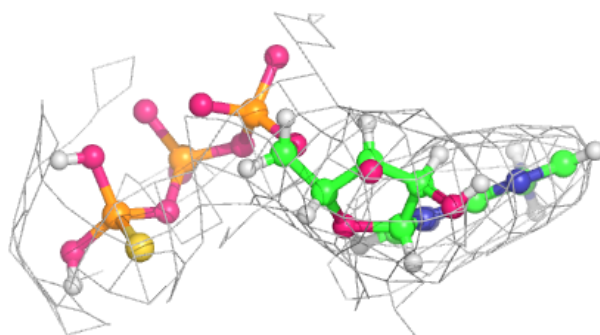
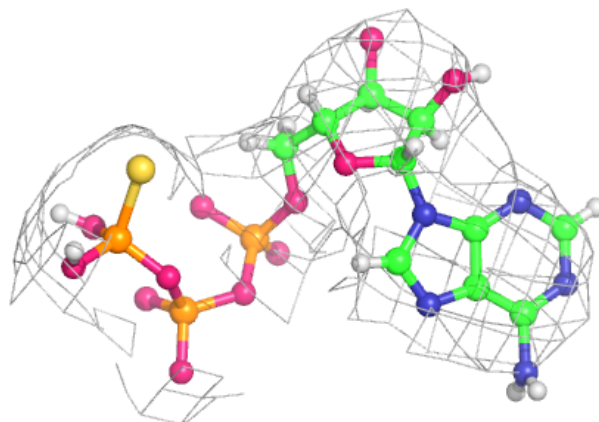


**Electron density around AGS D 901:**

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

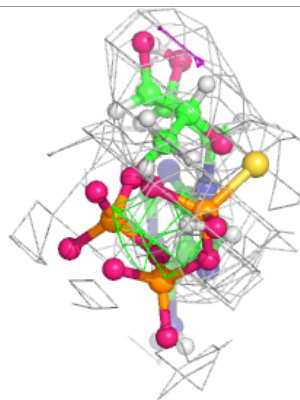
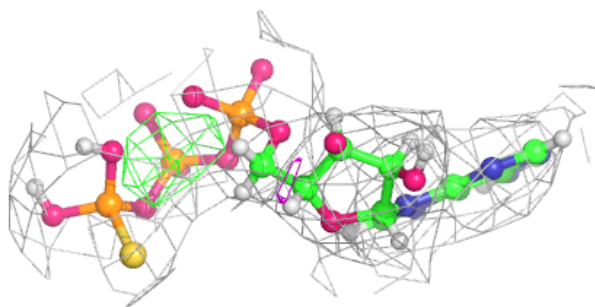
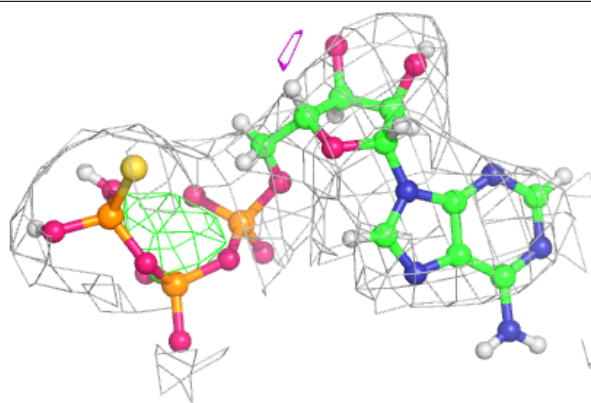
**Electron density around AGS C 901:**

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

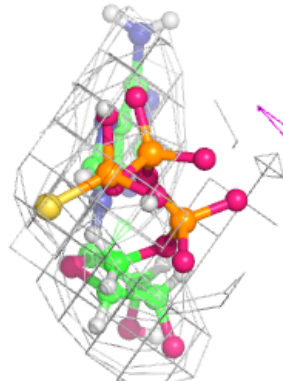
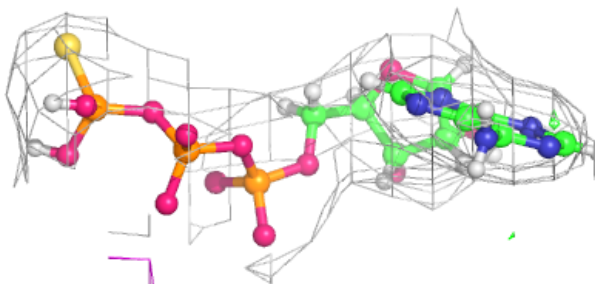
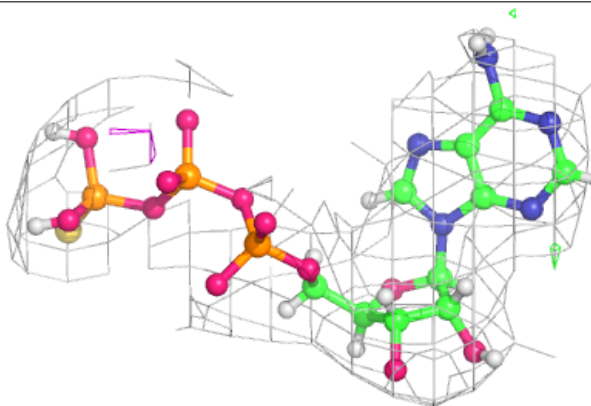


**Electron density around AGS A 901:**

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

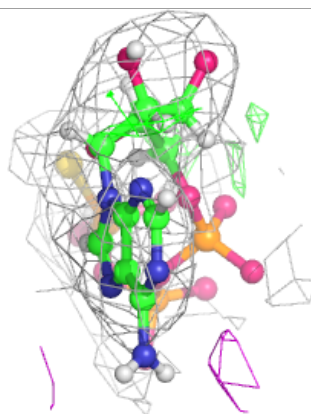
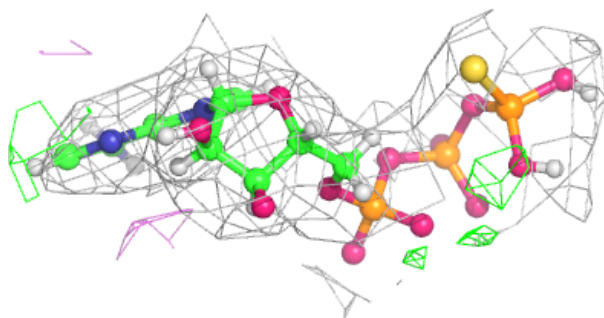
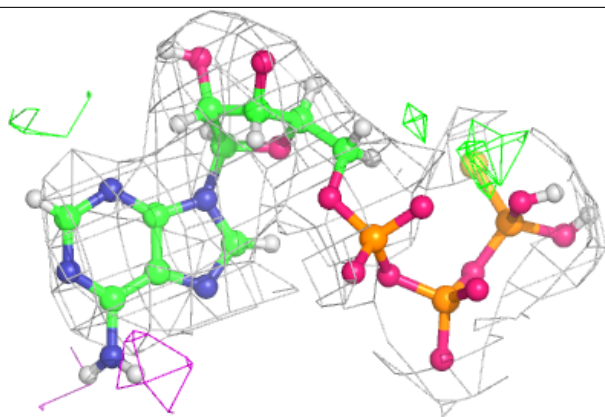
**Electron density around AGS D 902:**

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

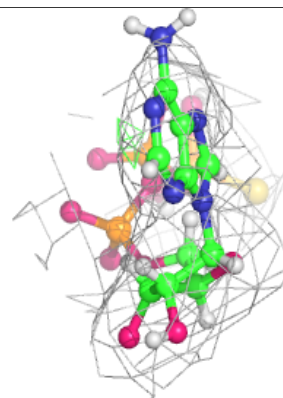
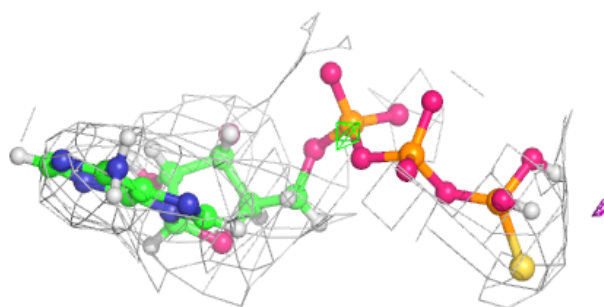
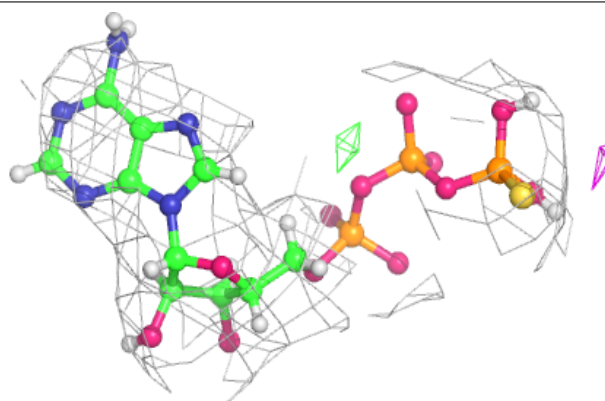


**Electron density around AGS F 901:**

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

**Electron density around AGS F 902:**

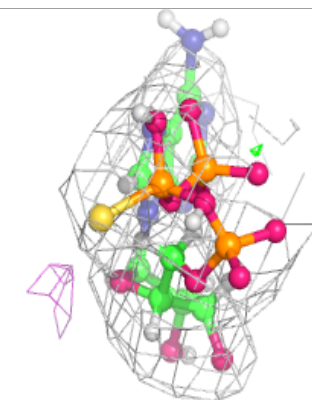
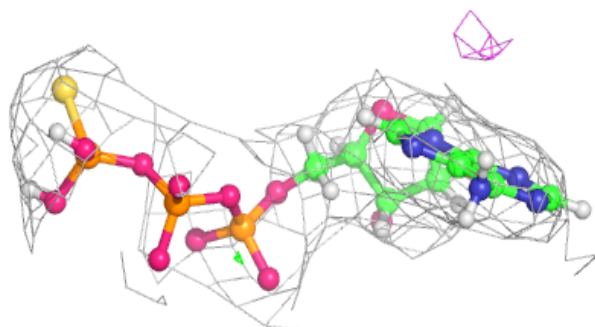
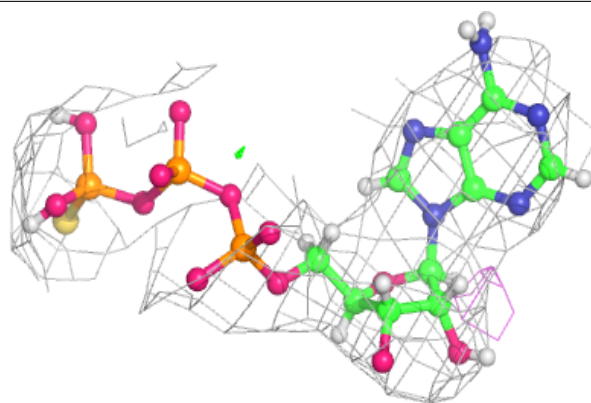
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



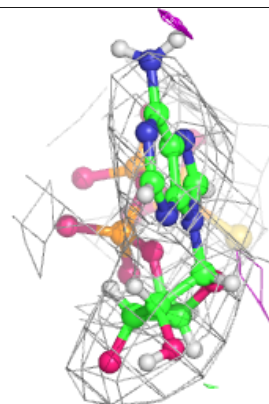
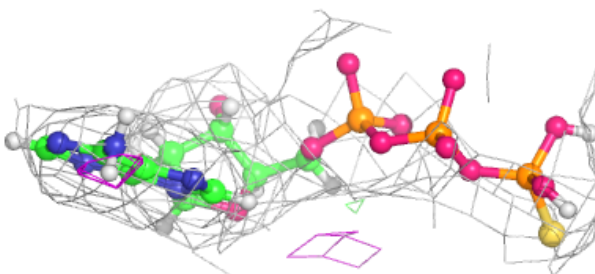
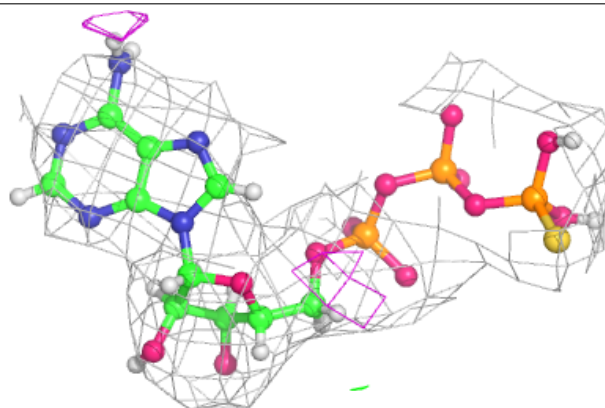


**Electron density around AGS E 902:**

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

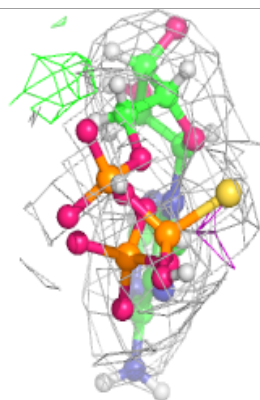
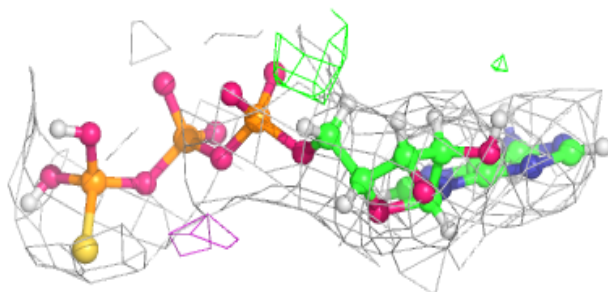
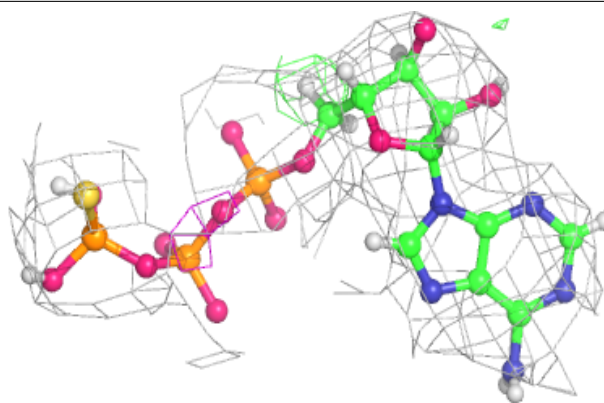
**Electron density around AGS C 902:**

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

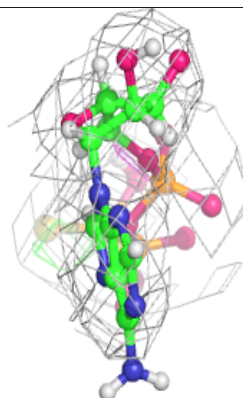
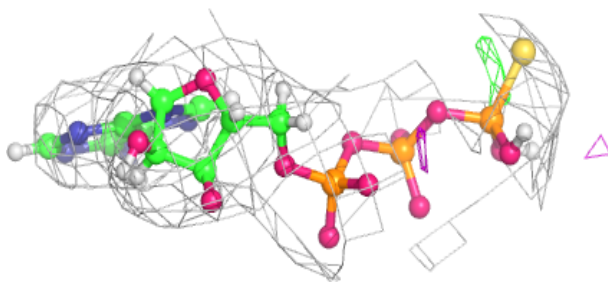
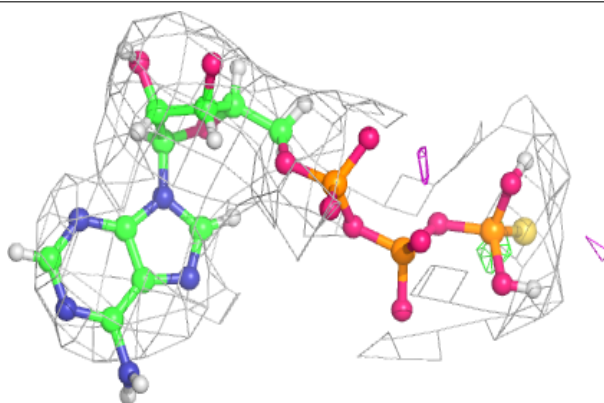


**Electron density around AGS B 902:**

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

**Electron density around AGS A 902:**

$2mF_o-DF_c$  (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.