



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 12:50 AM BST

PDB ID : 5C1B  
Title : p97-delta709-728 in complex with a UFD1-SHP peptide  
Authors : Haenzelmann, P.; Schindelin, H.  
Deposited on : 2015-06-13  
Resolution : 3.08 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.

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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 : 2.13.1  
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) : 2.13.1

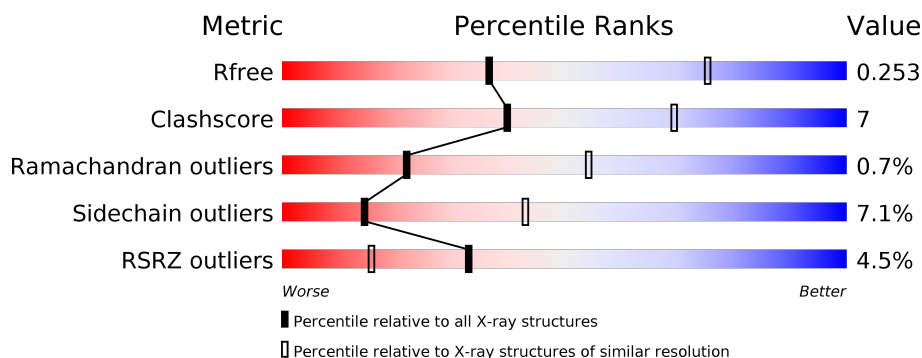
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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>4%</div> <div> <div></div> <div>70%</div> <div>19%</div> <div>8%</div> </div> </div>
1	B	785	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>8%</div> </div> </div>
1	C	785	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>8%</div> </div> </div>
1	D	785	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>8%</div> </div> </div>
1	E	785	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>8%</div> </div> </div>
1	F	785	<div> <div>9%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	U	21	<p>10% 24% 24% 52%</p>
2	V	21	<p>5% 24% 29% 48%</p>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 69385 atoms, of which 34726 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	724	Total	C	H	N	O	S	0	0	0
			11417	3572	5739	1003	1073	30			
1	B	724	Total	C	H	N	O	S	0	0	0
			11426	3572	5748	1003	1073	30			
1	C	724	Total	C	H	N	O	S	0	0	0
			11427	3572	5749	1003	1073	30			
1	D	724	Total	C	H	N	O	S	0	0	0
			11427	3572	5749	1003	1073	30			
1	E	724	Total	C	H	N	O	S	0	0	0
			11426	3572	5748	1003	1073	30			
1	F	724	Total	C	H	N	O	S	0	0	0
			11427	3572	5749	1003	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

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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

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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

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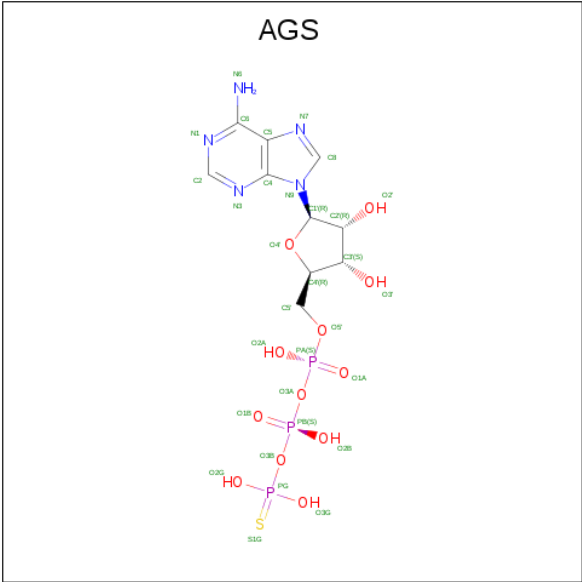
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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLU	deletion	UNP P55072
F	?	-	ARG	deletion	UNP P55072
F	?	-	GLU	deletion	UNP P55072
F	?	-	ARG	deletion	UNP P55072
F	?	-	GLN	deletion	UNP P55072
F	?	-	THR	deletion	UNP P55072
F	?	-	ASN	deletion	UNP 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 a protein called Ubiquitin fusion degradation protein 1 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	11	Total	C	H	N	O	0	0	0
			125	53	40	18	14			
2	U	10	Total	C	H	N	O	0	0	0
			106	44	32	17	13			

- Molecule 3 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
3	A	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	A	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	B	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	B	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	C	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	C	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	D	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	D	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	E	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	E	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	F	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
3	F	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

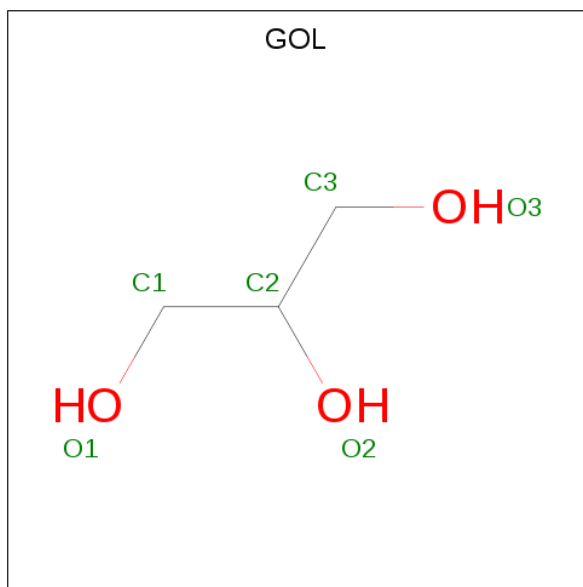


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	2	Total Mg 2 2	0	0
4	E	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0
4	C	2	Total Mg 2 2	0	0
4	A	2	Total Mg 2 2	0	0
4	F	2	Total Mg 2 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	1	Total	C	H	O	0	0
			14	3	8	3		
6	F	1	Total	C	H	O	0	0
			14	3	8	3		

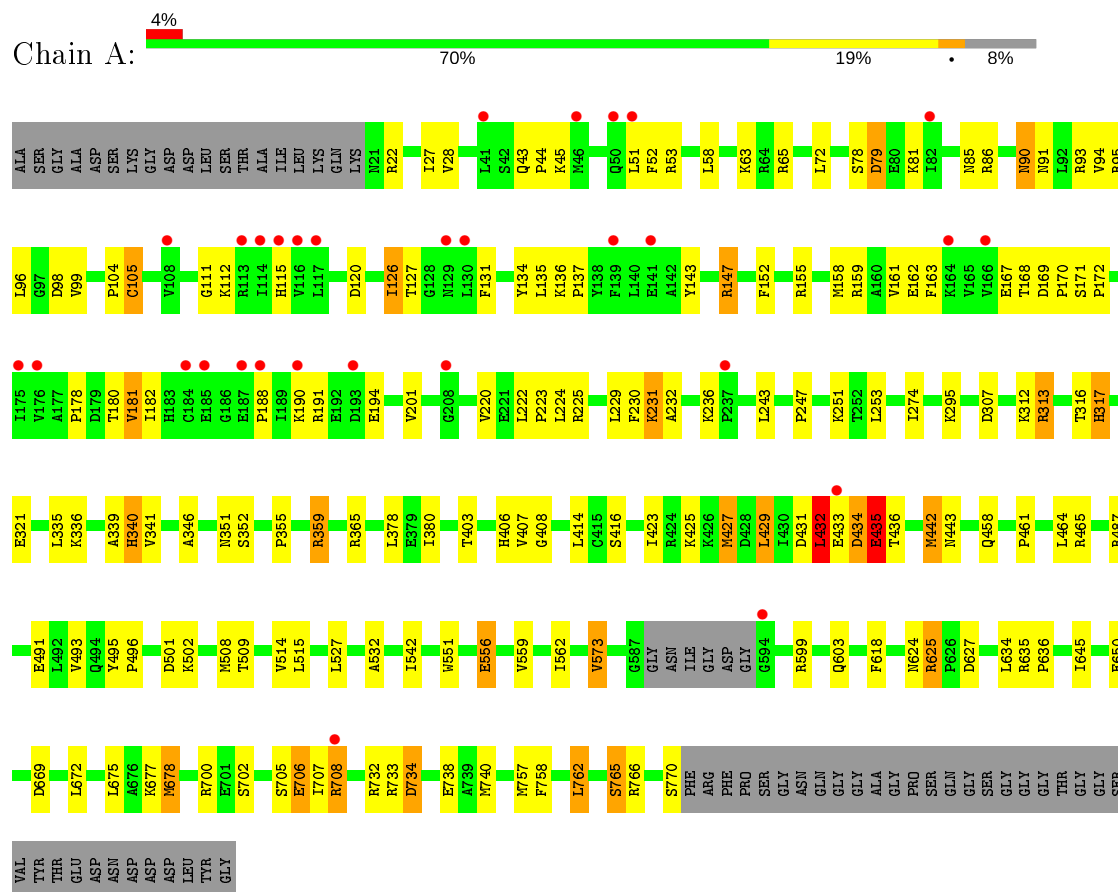
- Molecule 7 is water.

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

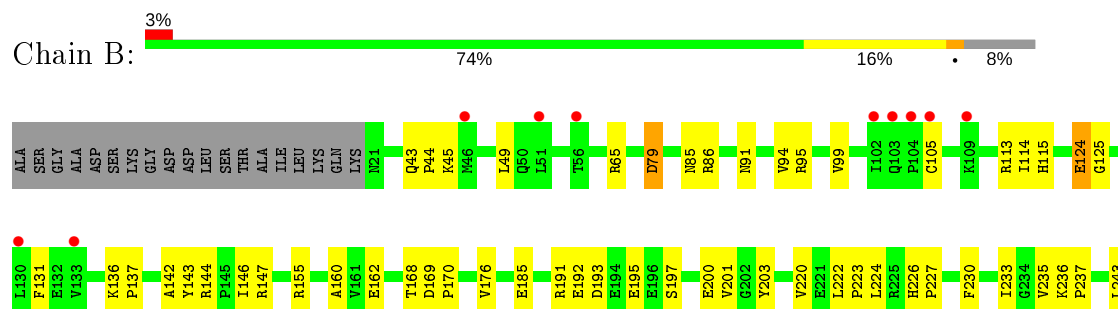
### 3 Residue-property plots [i](#)

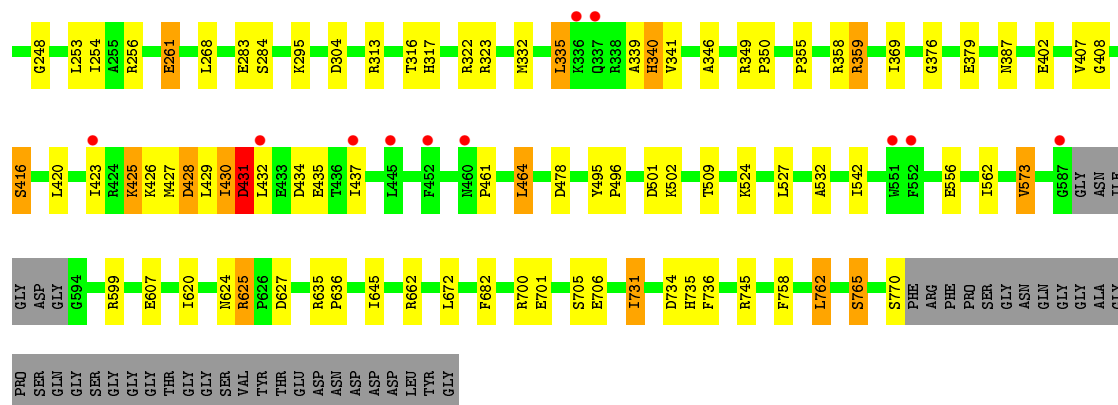
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Transitional endoplasmic reticulum ATPase

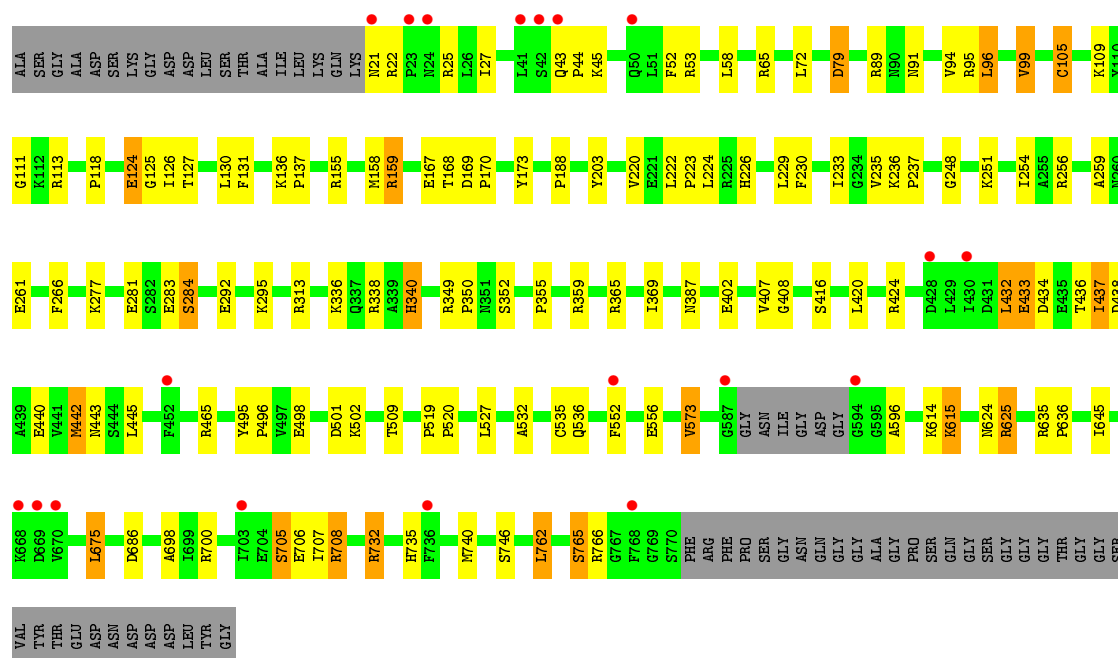
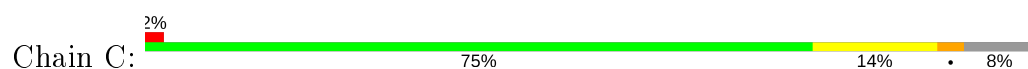


#### • Molecule 1: Transitional endoplasmic reticulum ATPase

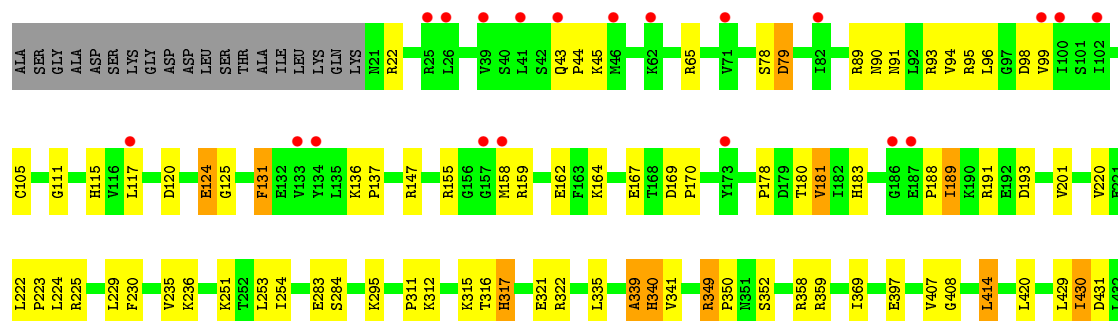
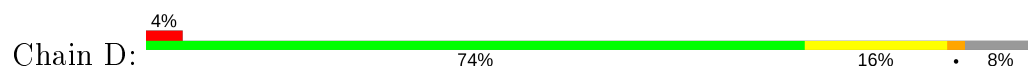


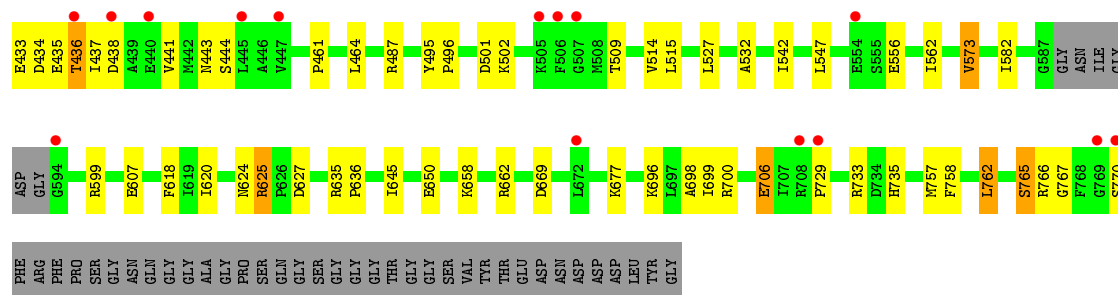


• Molecule 1: Transitional endoplasmic reticulum ATPase

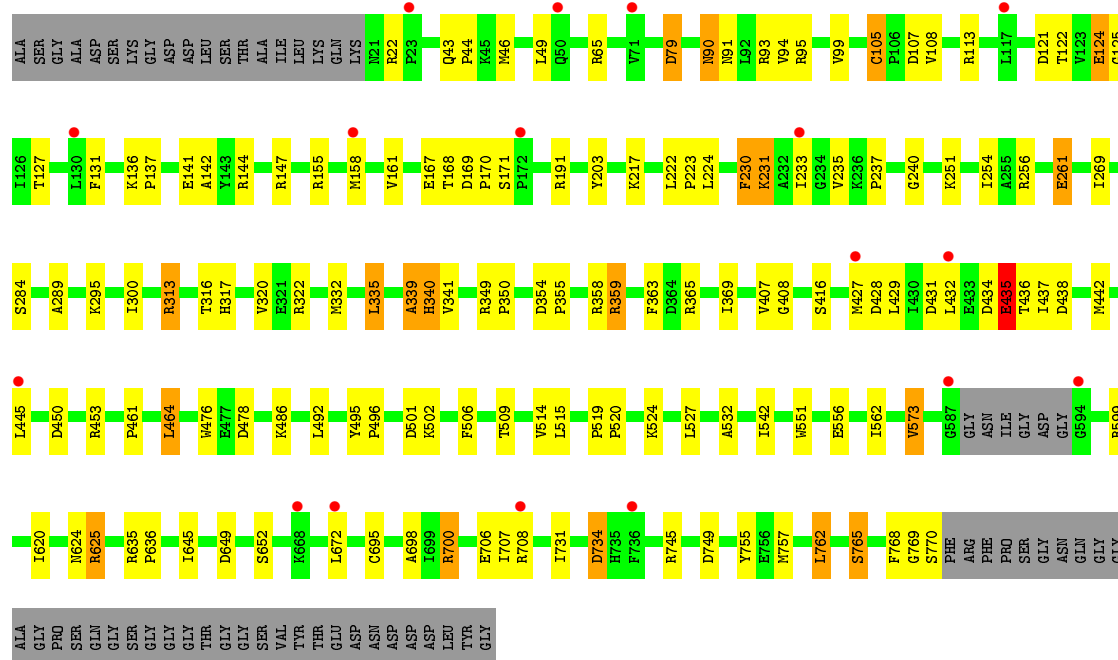


• Molecule 1: Transitional endoplasmic reticulum ATPase

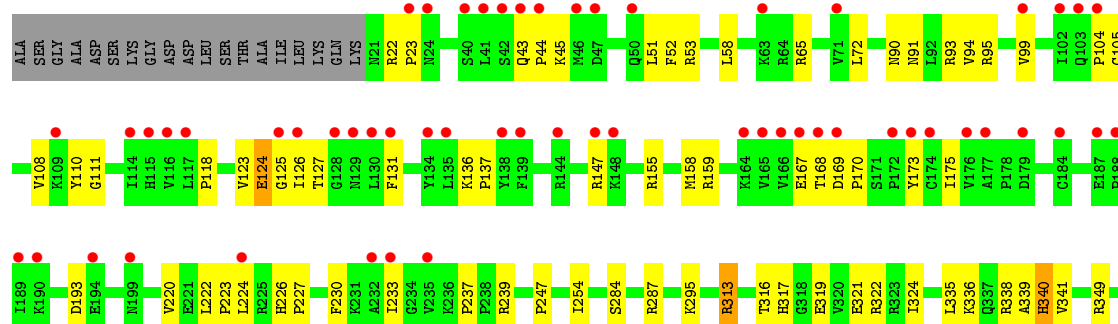
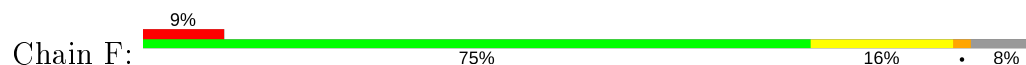


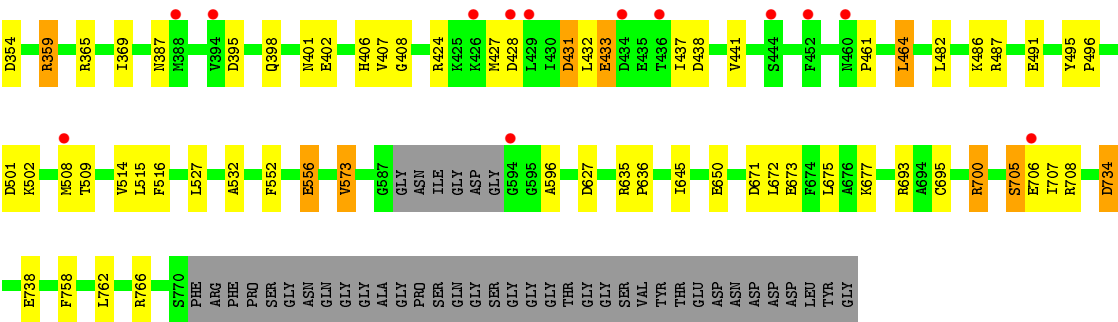


• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase





● Molecule 2: Ubiquitin fusion degradation protein 1 homolog



● Molecule 2: Ubiquitin fusion degradation protein 1 homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.72Å 180.66Å 254.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.14 – 3.08 49.14 – 3.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.14-3.08) 100.0 (49.14-3.08)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.198 , 0.240 0.210 , 0.253	Depositor DCC
$R_{free}$ test set	6055 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	108.5	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 85.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	69385	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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: GOL, 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	0/5771	0.44	0/7791
1	B	0.22	0/5771	0.43	0/7791
1	C	0.22	0/5771	0.44	0/7791
1	D	0.23	0/5771	0.44	0/7791
1	E	0.22	0/5771	0.42	0/7791
1	F	0.22	0/5771	0.44	0/7791
2	U	0.25	0/74	0.51	0/96
2	V	0.26	0/86	0.56	0/112
All	All	0.22	0/34786	0.44	0/46954

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	5678	5739	5749	107	1
1	B	5678	5748	5749	84	0
1	C	5678	5749	5749	74	1
1	D	5678	5749	5749	88	1
1	E	5678	5748	5749	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	5678	5749	5749	74	1
2	U	74	32	72	17	0
2	V	85	40	81	22	0
3	A	62	26	24	4	0
3	B	62	26	24	1	0
3	C	62	26	24	3	0
3	D	62	26	24	1	0
3	E	62	26	24	4	0
3	F	62	26	24	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	F	12	16	16	0	0
7	A	5	0	0	1	0
7	B	5	0	0	2	0
7	C	5	0	0	1	0
7	D	5	0	0	0	0
7	E	5	0	0	1	0
7	F	5	0	0	1	0
All	All	34659	34726	34807	510	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 510 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:OE1	1:A:191:ARG:NH2	1.83	1.10
2:V:227:ALA:HB1	2:V:228:PHE:CD1	2.02	0.94
1:D:162:GLU:OE1	1:D:191:ARG:NH2	2.04	0.91
1:B:429:LEU:O	1:B:431:ASP:N	2.04	0.90
1:D:181:VAL:HA	2:V:233:ASN:HB3	1.55	0.89

All (2) 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:C:284:SER:OG	1:F:671:ASP:OD2[3_555]	2.02	0.18
1:A:112:LYS:NZ	1:D:397:GLU:OE1[1_455]	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	720/785 (92%)	690 (96%)	25 (4%)	5 (1%)	22	54
1	B	720/785 (92%)	696 (97%)	20 (3%)	4 (1%)	25	57
1	C	720/785 (92%)	698 (97%)	20 (3%)	2 (0%)	41	71
1	D	720/785 (92%)	697 (97%)	21 (3%)	2 (0%)	41	71
1	E	720/785 (92%)	695 (96%)	20 (3%)	5 (1%)	22	54
1	F	720/785 (92%)	693 (96%)	23 (3%)	4 (1%)	25	57
2	U	8/21 (38%)	1 (12%)	3 (38%)	4 (50%)	0	0
2	V	9/21 (43%)	2 (22%)	3 (33%)	4 (44%)	0	0
All	All	4337/4752 (91%)	4172 (96%)	135 (3%)	30 (1%)	22	54

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	HIS
1	B	428	ASP
1	B	430	ILE
1	B	431	ASP
1	C	706	GLU

### 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	617/658 (94%)	561 (91%)	56 (9%)	9	31
1	B	617/658 (94%)	583 (94%)	34 (6%)	21	52
1	C	617/658 (94%)	563 (91%)	54 (9%)	10	34
1	D	617/658 (94%)	573 (93%)	44 (7%)	14	43
1	E	617/658 (94%)	576 (93%)	41 (7%)	16	45
1	F	617/658 (94%)	584 (95%)	33 (5%)	22	53
2	U	7/14 (50%)	6 (86%)	1 (14%)	3	13
2	V	8/14 (57%)	6 (75%)	2 (25%)	0	1
All	All	3717/3976 (94%)	3452 (93%)	265 (7%)	14	43

5 of 265 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	365	ARG
1	D	99	VAL
1	F	349	ARG
1	C	432	LEU
1	C	614	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	340	HIS
1	D	90	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 18 are monoatomic - leaving 14 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$
3	AGS	D	903	4	26,33,33	1.46	5 (19%)	26,52,52	1.69	6 (23%)
6	GOL	F	907	-	5,5,5	0.37	0	5,5,5	0.24	0
3	AGS	D	902	4	26,33,33	1.47	5 (19%)	26,52,52	1.73	5 (19%)
3	AGS	C	903	4	26,33,33	1.47	5 (19%)	26,52,52	1.68	4 (15%)
3	AGS	B	901	4	26,33,33	1.44	5 (19%)	26,52,52	1.70	4 (15%)
3	AGS	B	902	4	26,33,33	1.45	6 (23%)	26,52,52	1.72	5 (19%)
3	AGS	F	901	4	26,33,33	1.43	5 (19%)	26,52,52	1.72	5 (19%)
3	AGS	F	902	4	26,33,33	1.47	6 (23%)	26,52,52	1.64	4 (15%)
3	AGS	A	902	4	26,33,33	1.45	5 (19%)	26,52,52	1.66	5 (19%)
3	AGS	C	902	4	26,33,33	1.49	6 (23%)	26,52,52	1.58	3 (11%)
3	AGS	A	901	4	26,33,33	1.48	6 (23%)	26,52,52	1.57	3 (11%)
6	GOL	F	906	-	5,5,5	0.41	0	5,5,5	0.21	0
3	AGS	E	902	4	26,33,33	1.46	5 (19%)	26,52,52	1.66	6 (23%)
3	AGS	E	901	4	26,33,33	1.51	7 (26%)	26,52,52	1.65	3 (11%)

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
3	AGS	D	903	4	-	9/17/38/38	0/3/3/3
6	GOL	F	907	-	-	2/4/4/4	-
3	AGS	D	902	4	-	5/17/38/38	0/3/3/3
3	AGS	C	903	4	-	7/17/38/38	0/3/3/3
3	AGS	B	901	4	-	7/17/38/38	0/3/3/3
3	AGS	B	902	4	-	7/17/38/38	0/3/3/3
3	AGS	F	901	4	-	4/17/38/38	0/3/3/3
3	AGS	F	902	4	-	4/17/38/38	0/3/3/3
3	AGS	A	902	4	-	3/17/38/38	0/3/3/3
3	AGS	C	902	4	-	4/17/38/38	0/3/3/3
3	AGS	A	901	4	-	3/17/38/38	0/3/3/3
6	GOL	F	906	-	-	2/4/4/4	-
3	AGS	E	902	4	-	6/17/38/38	0/3/3/3
3	AGS	E	901	4	-	5/17/38/38	0/3/3/3

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	901	AGS	C2-N3	3.28	1.37	1.32
3	D	903	AGS	C2-N3	3.19	1.37	1.32
3	C	903	AGS	C2-N3	3.17	1.37	1.32
3	E	902	AGS	C2-N3	3.17	1.37	1.32
3	C	902	AGS	C2-N3	3.14	1.37	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	AGS	N3-C2-N1	-5.76	119.67	128.68
3	A	902	AGS	N3-C2-N1	-5.68	119.80	128.68
3	B	902	AGS	N3-C2-N1	-5.58	119.95	128.68
3	C	903	AGS	N3-C2-N1	-5.56	119.98	128.68
3	F	902	AGS	N3-C2-N1	-5.56	119.99	128.68

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	903	AGS	C5'-O5'-PA-O3A
3	A	902	AGS	PB-O3B-PG-O2G

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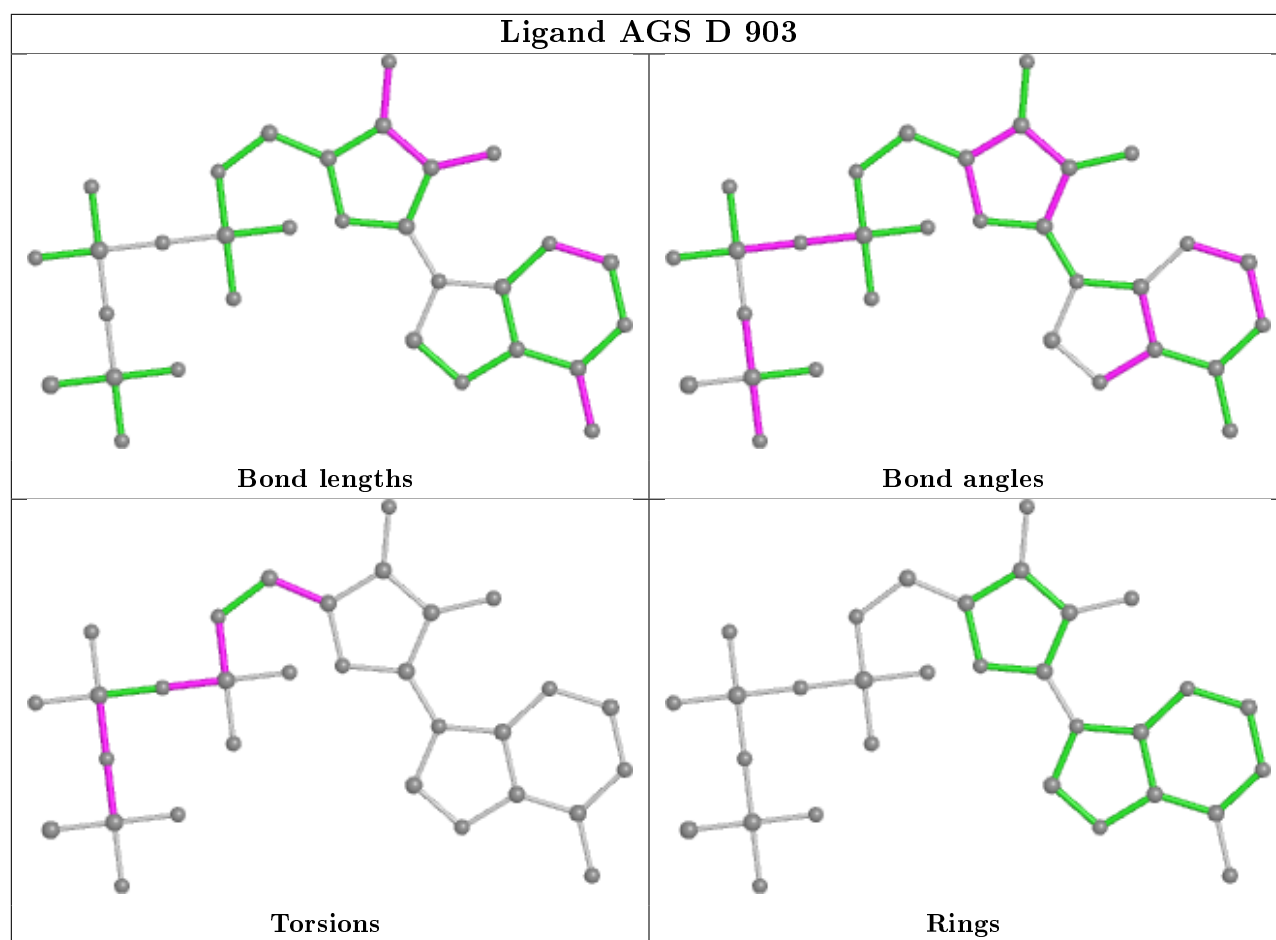
Mol	Chain	Res	Type	Atoms
3	A	902	AGS	PB-O3B-PG-O3G
3	D	903	AGS	PB-O3B-PG-O2G
3	D	903	AGS	PB-O3B-PG-O3G

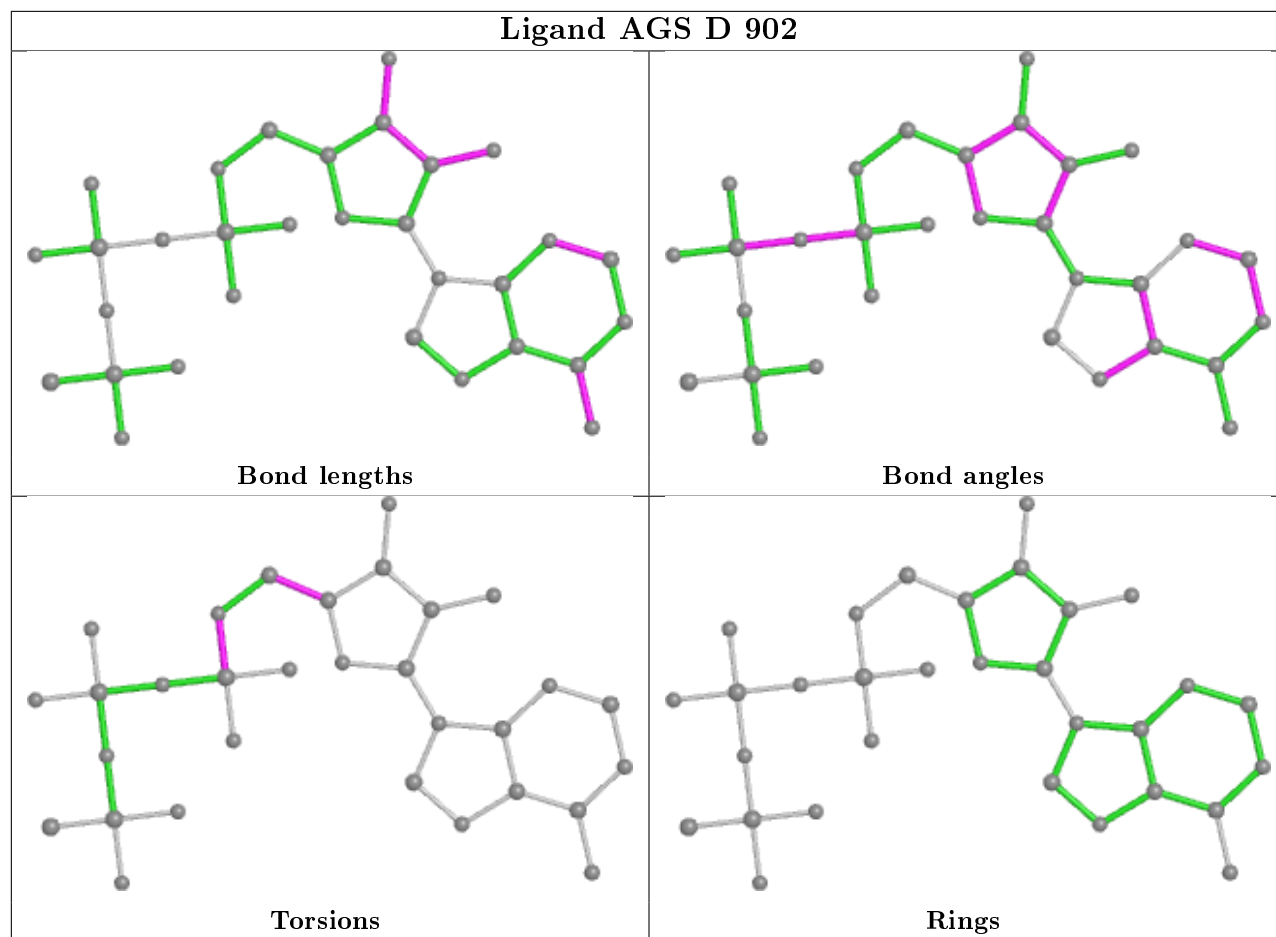
There are no ring outliers.

9 monomers are involved in 17 short contacts:

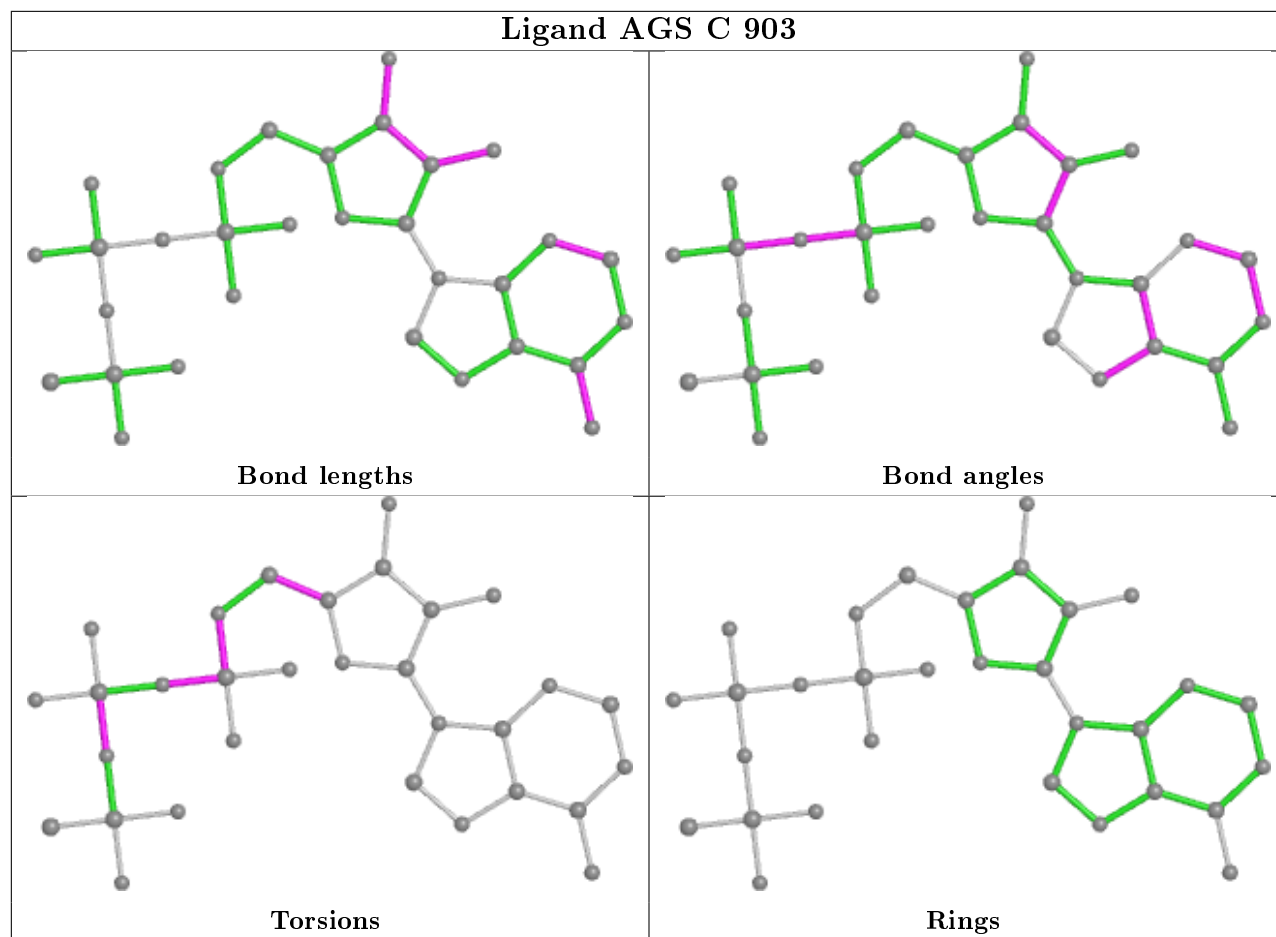
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	902	AGS	1	0
3	C	903	AGS	1	0
3	B	902	AGS	1	0
3	F	901	AGS	3	0
3	F	902	AGS	1	0
3	C	902	AGS	2	0
3	A	901	AGS	4	0
3	E	902	AGS	1	0
3	E	901	AGS	3	0

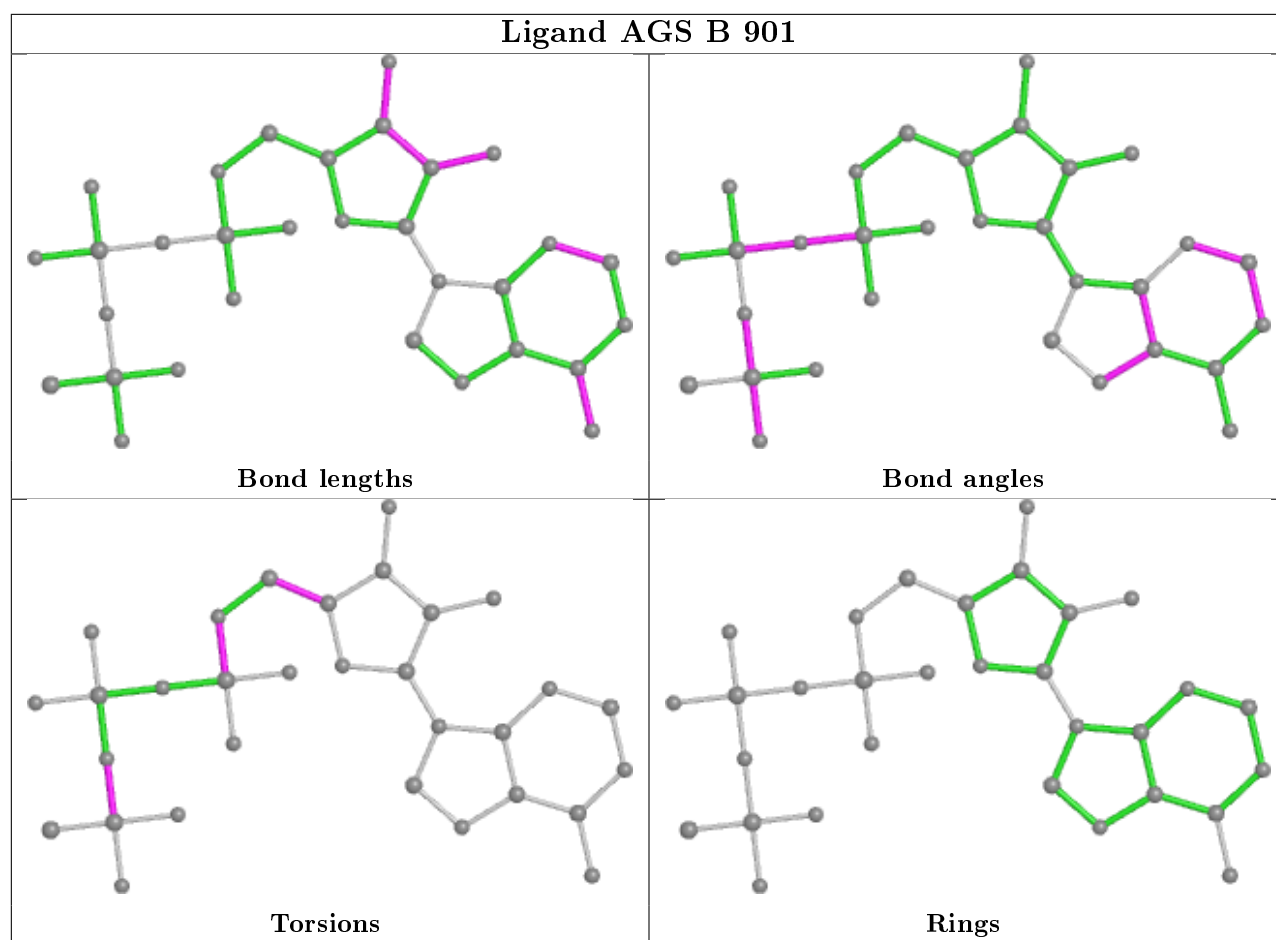
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

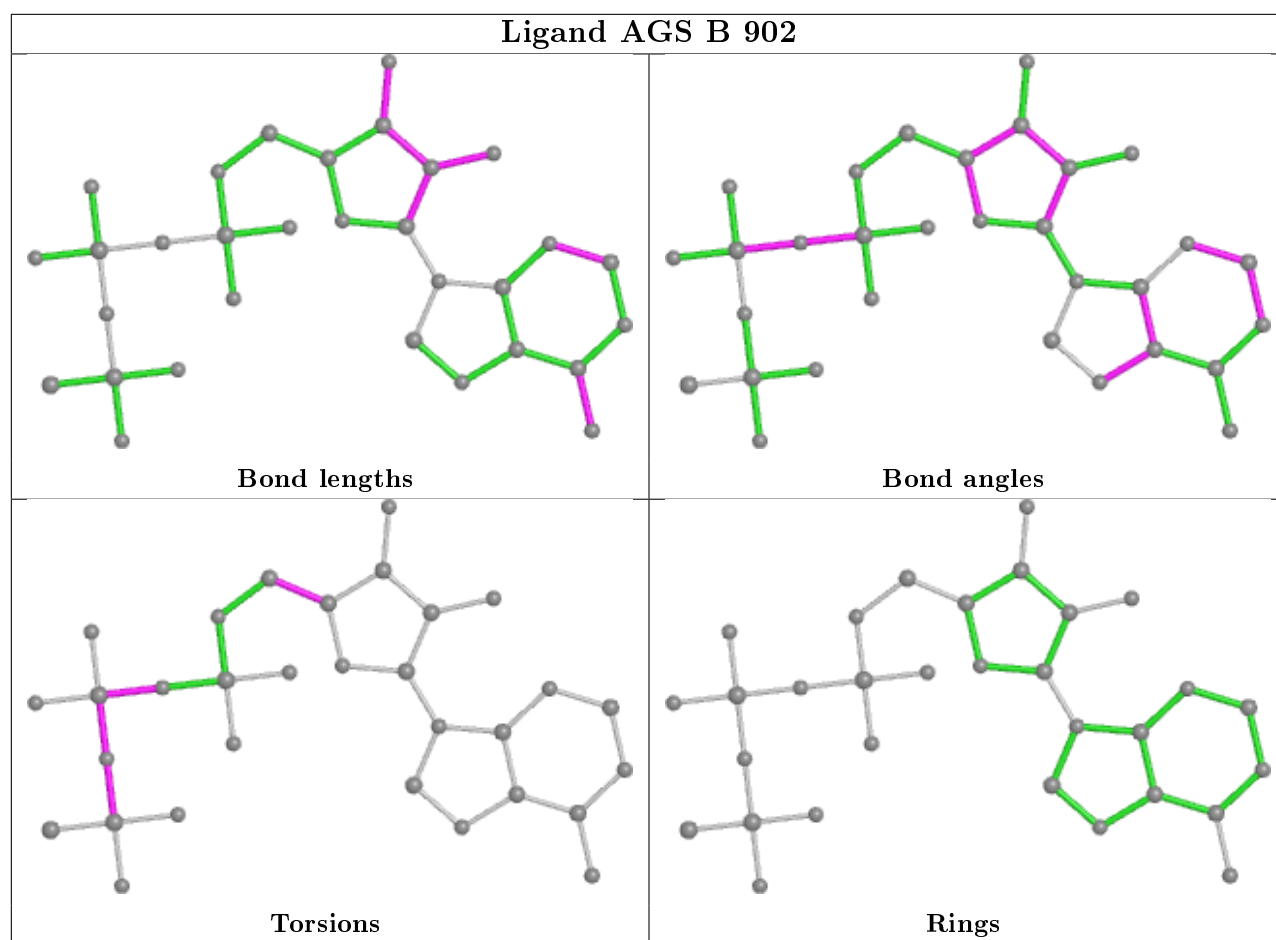




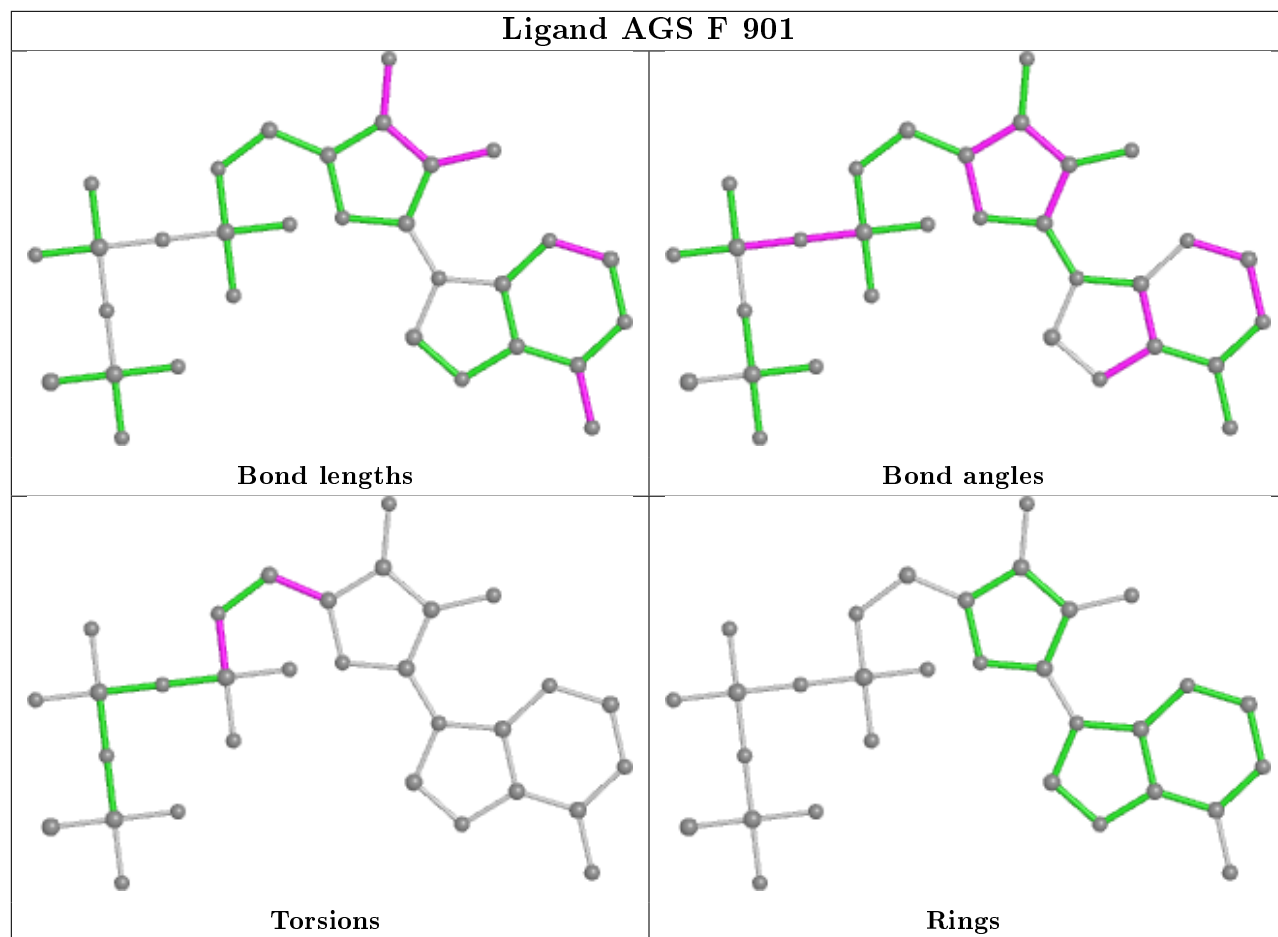




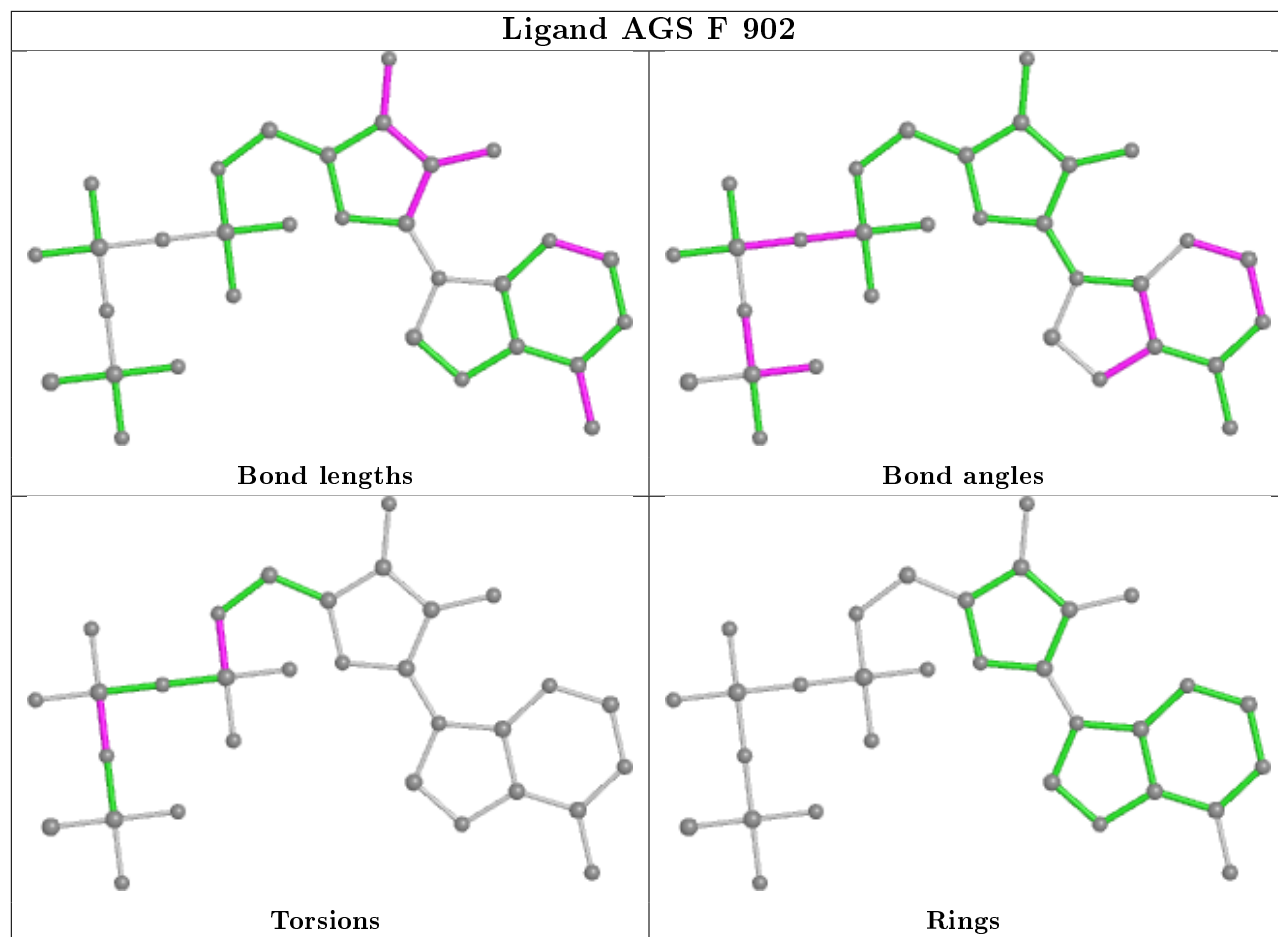


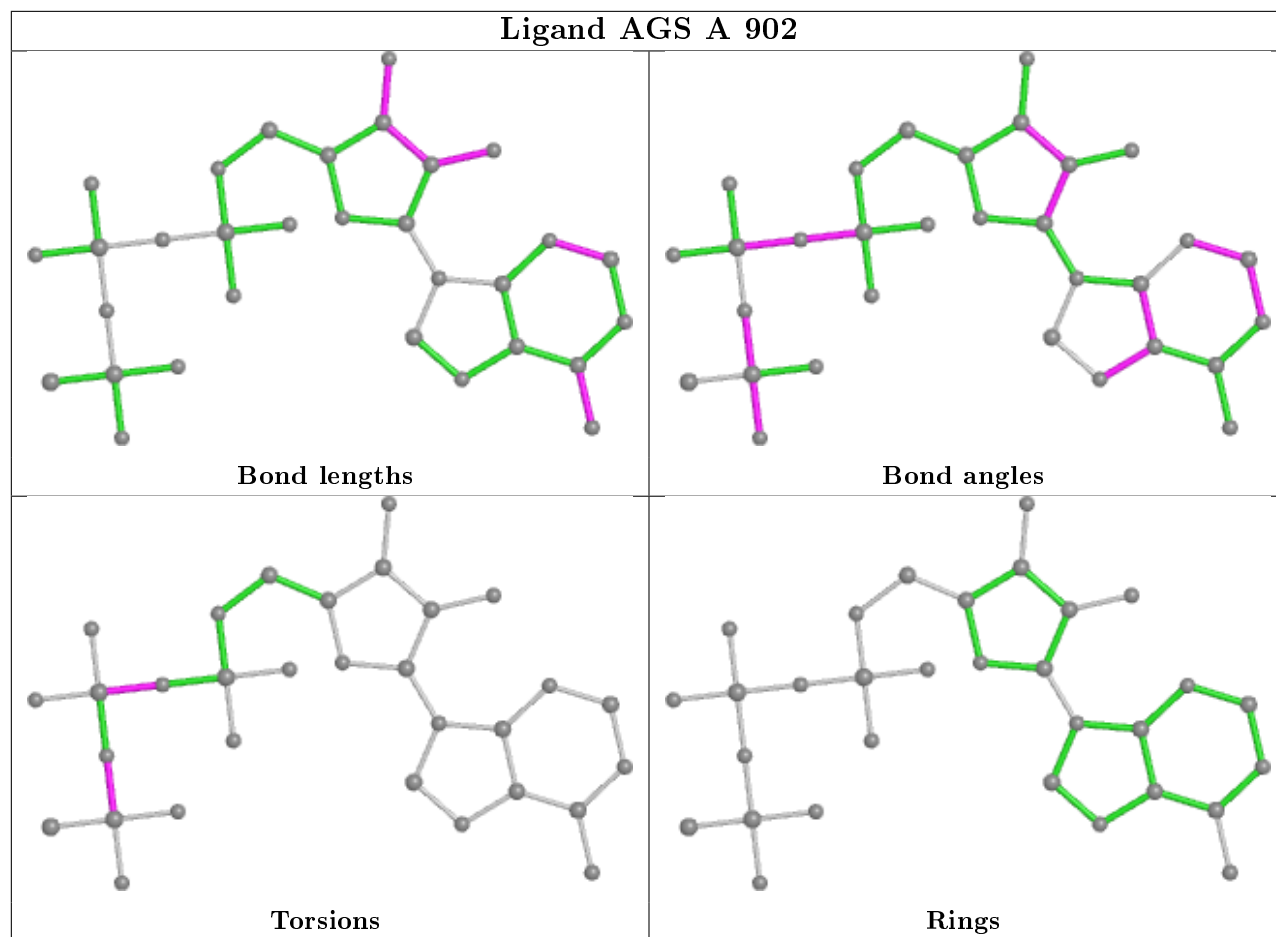


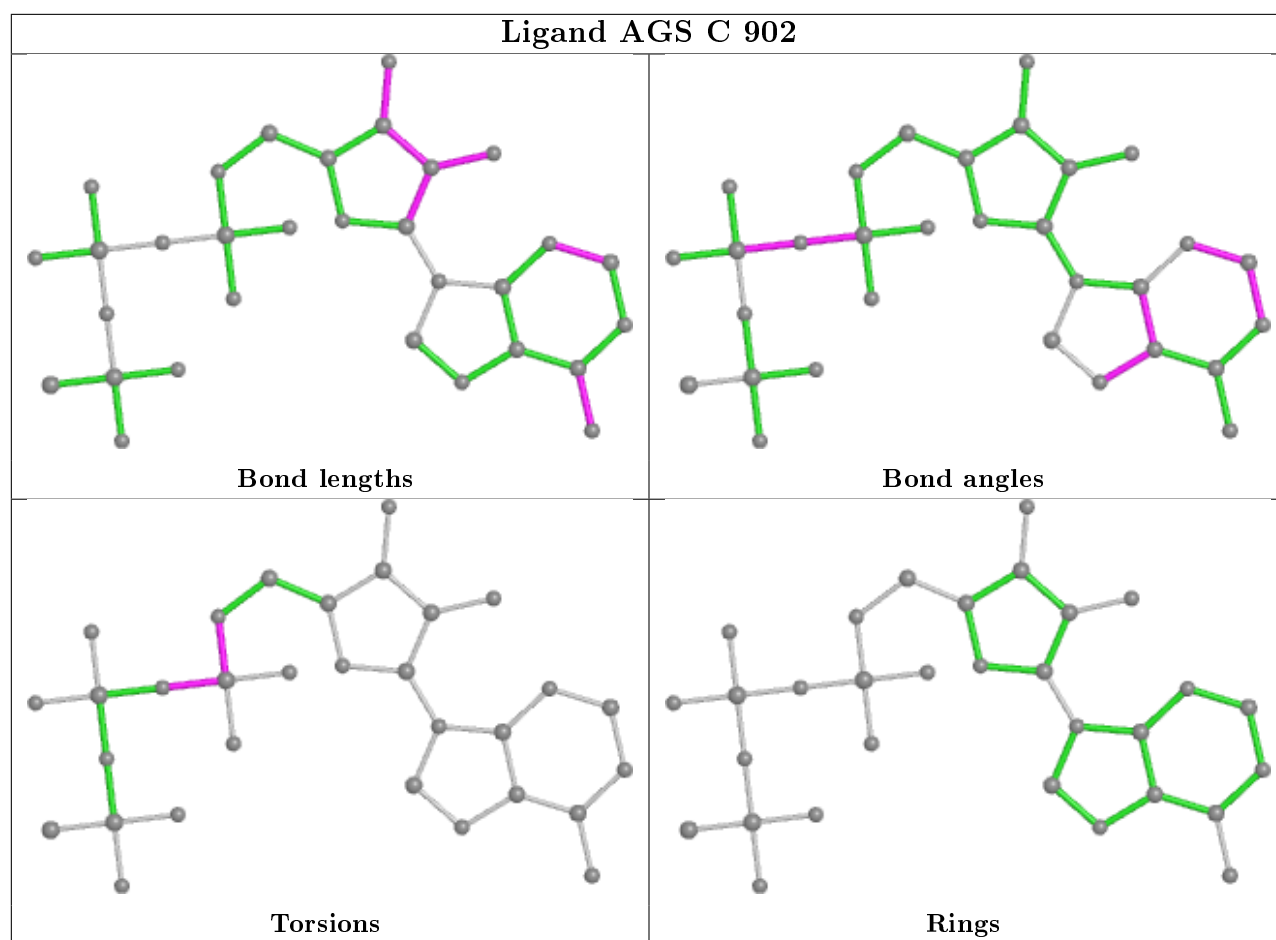
## Ligand AGS F 901

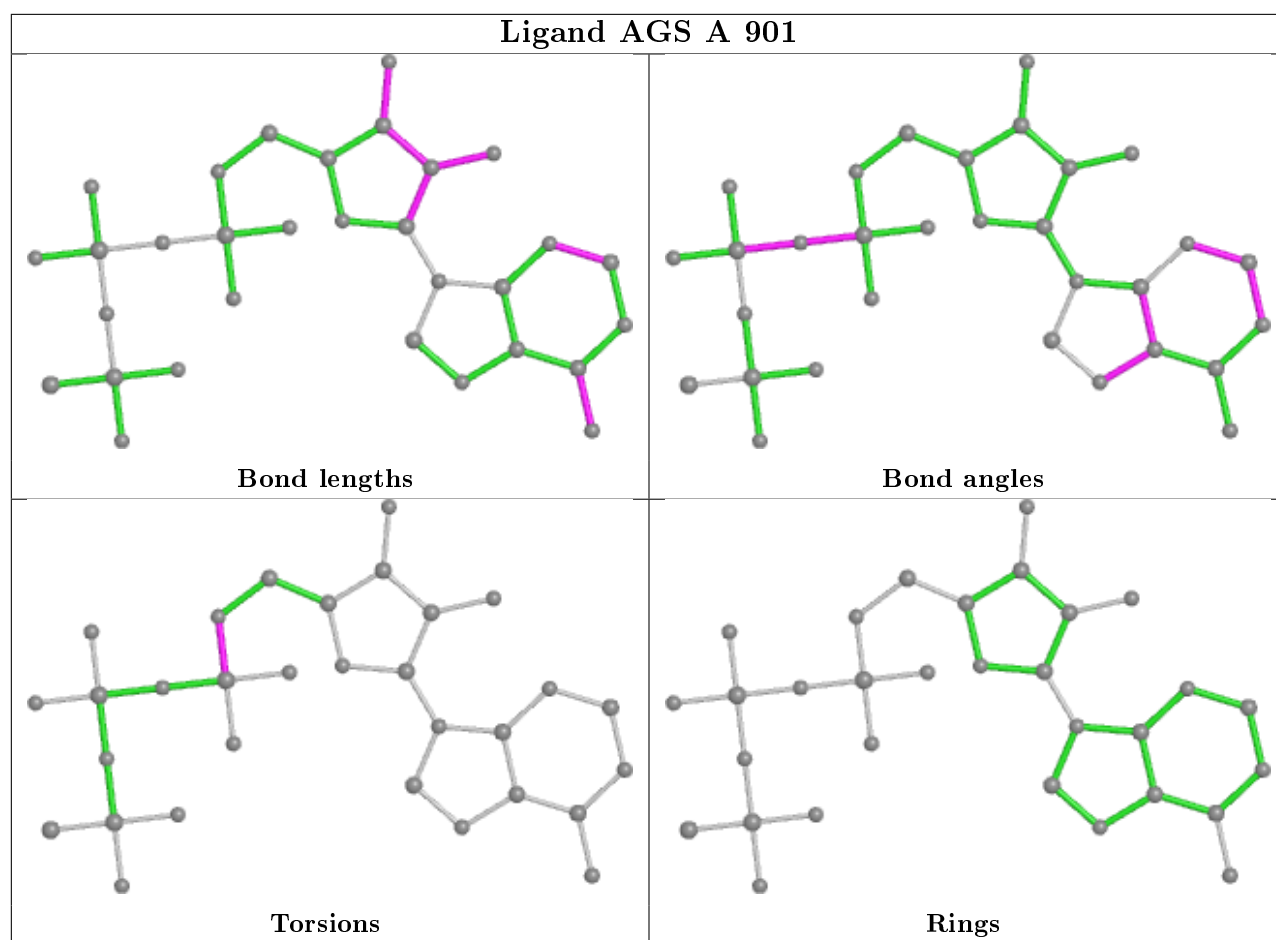


## Ligand AGS F 902



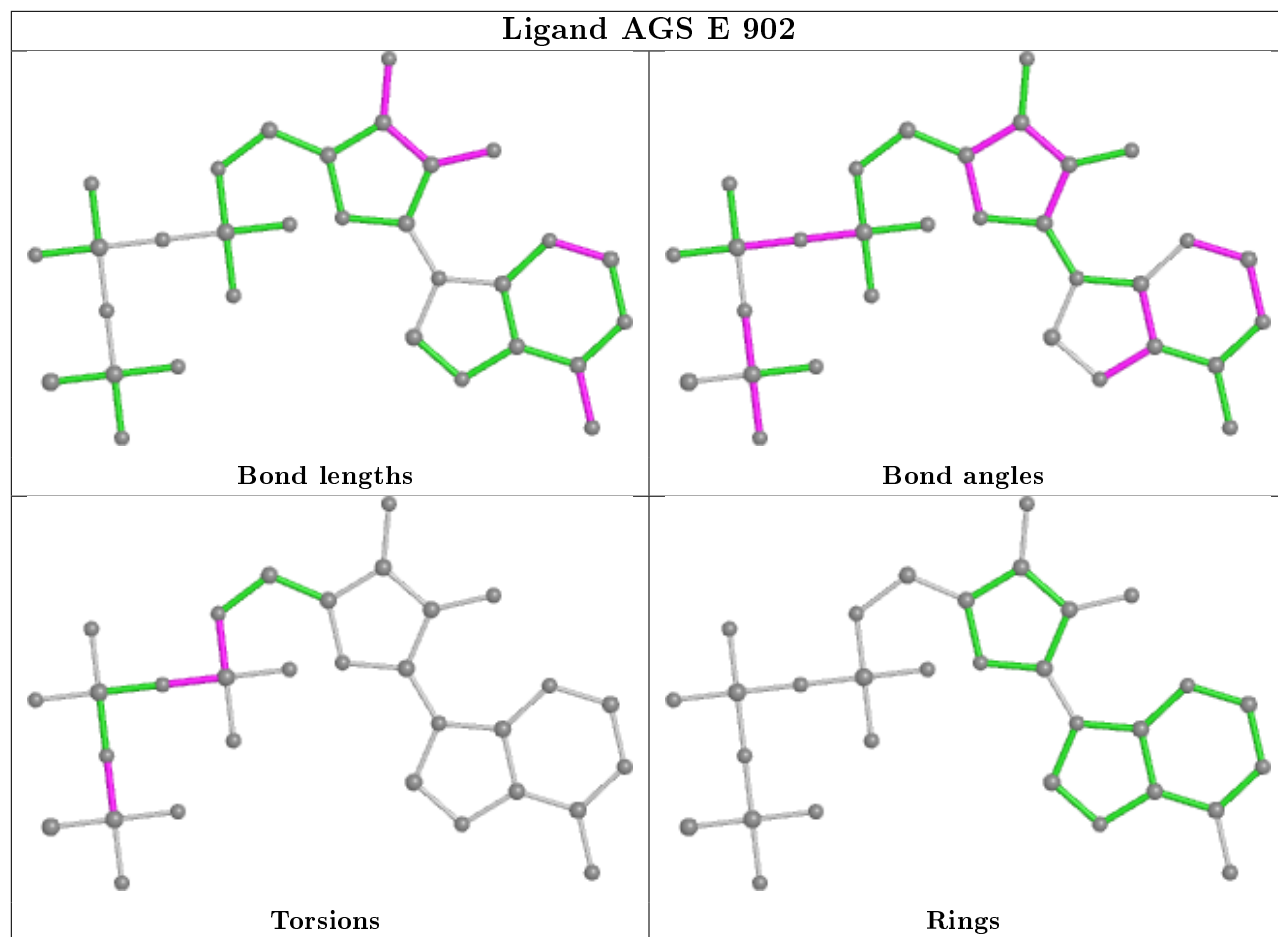


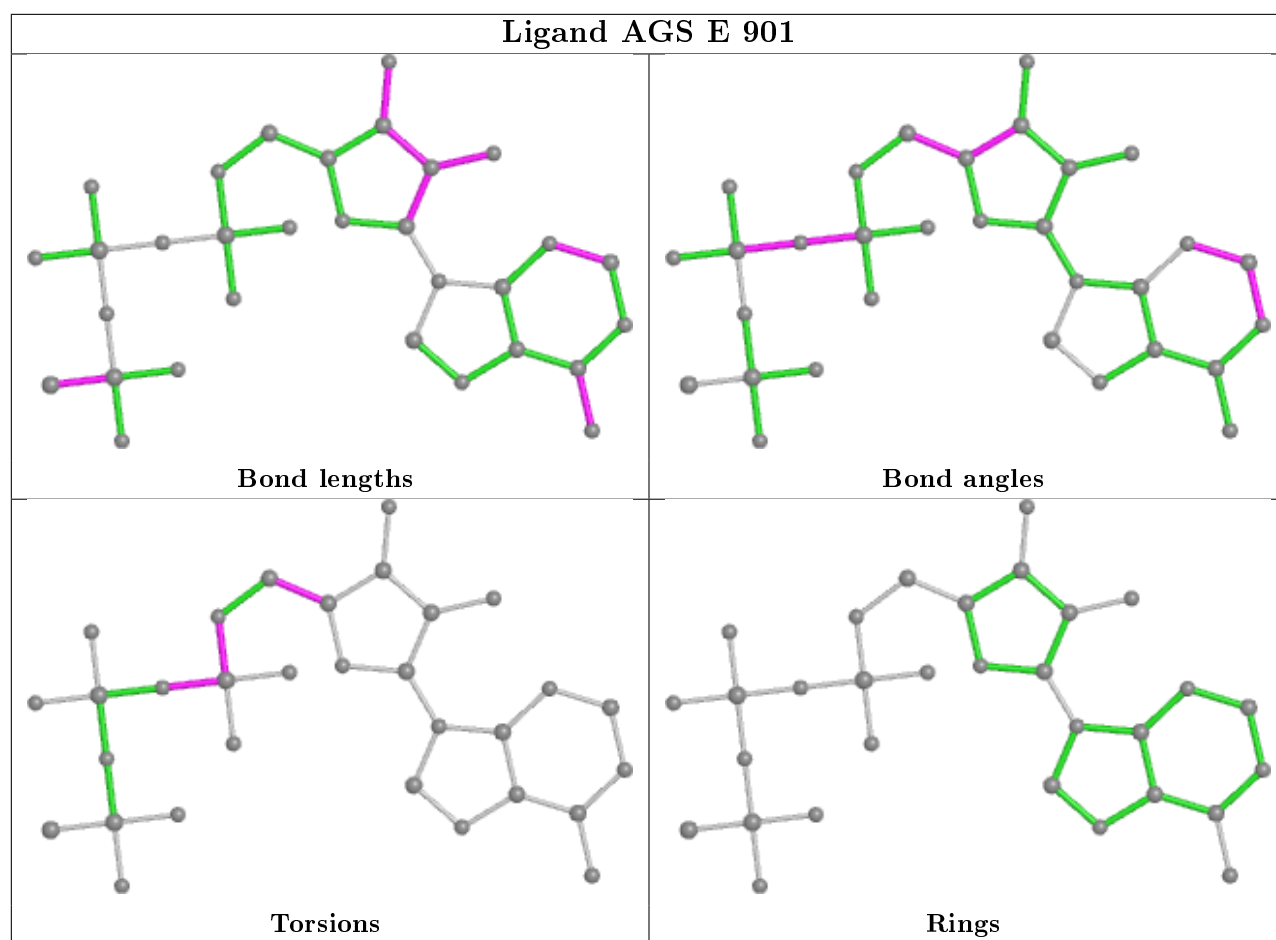






## Ligand AGS E 902





## 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, 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	724/785 (92%)	0.36	30 (4%) 37 18	69, 126, 205, 276	0
1	B	724/785 (92%)	0.15	21 (2%) 51 27	66, 118, 184, 264	0
1	C	724/785 (92%)	0.19	19 (2%) 56 31	55, 121, 199, 301	0
1	D	724/785 (92%)	0.25	35 (4%) 30 14	68, 130, 211, 317	0
1	E	724/785 (92%)	0.17	17 (2%) 60 37	75, 121, 192, 287	0
1	F	724/785 (92%)	0.52	70 (9%) 7 2	68, 131, 258, 320	0
2	U	10/21 (47%)	0.80	2 (20%) 1 0	170, 229, 262, 283	0
2	V	11/21 (52%)	1.04	1 (9%) 9 3	167, 186, 232, 328	0
All	All	4365/4752 (91%)	0.28	195 (4%) 33 16	55, 124, 217, 328	0

The worst 5 of 195 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	164	LYS	7.3
1	F	166	VAL	7.1
1	F	116	VAL	6.6
1	F	117	LEU	6.6
1	A	139	PHE	5.7

### 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 monosaccharides in this entry.

## 6.4 Ligands ⓘ

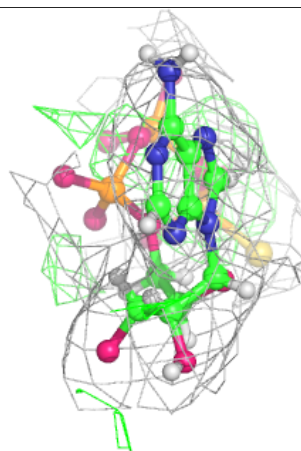
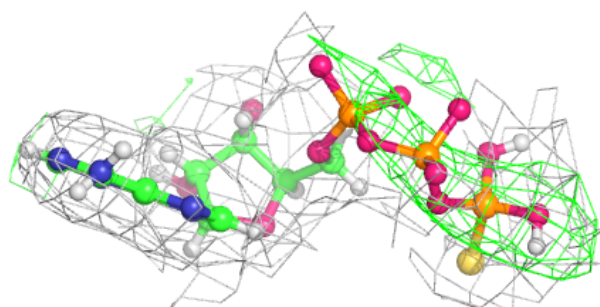
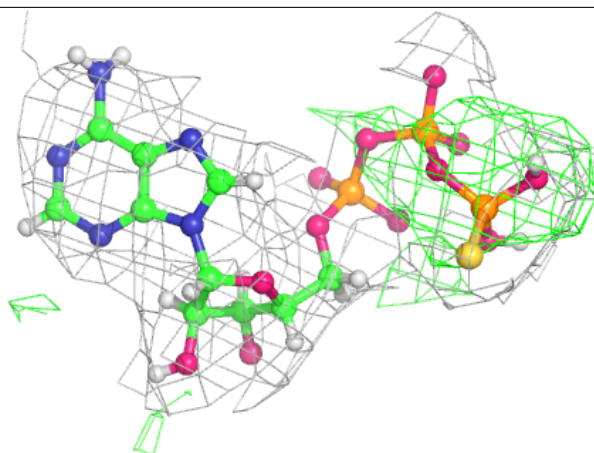
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
5	CL	C	901	1/1	0.70	0.31	130,130,130,130	0
5	CL	D	901	1/1	0.73	0.31	117,117,117,117	0
4	MG	A	903	1/1	0.78	0.19	243,243,243,243	0
5	CL	E	905	1/1	0.80	0.36	118,118,118,118	0
6	GOL	F	906	6/6	0.81	0.38	108,130,150,155	0
5	CL	A	905	1/1	0.84	0.32	98,98,98,98	0
4	MG	D	905	1/1	0.88	0.28	100,100,100,100	0
5	CL	B	905	1/1	0.89	0.28	105,105,105,105	0
4	MG	B	903	1/1	0.89	0.17	139,139,139,139	0
5	CL	F	905	1/1	0.91	0.36	109,109,109,109	0
4	MG	C	904	1/1	0.92	0.29	111,111,111,111	0
3	AGS	F	902	31/31	0.92	0.28	55,88,149,575	0
3	AGS	E	902	31/31	0.94	0.23	57,97,116,136	0
3	AGS	F	901	31/31	0.94	0.30	83,125,164,219	0
6	GOL	F	907	6/6	0.94	0.24	92,114,131,144	0
3	AGS	B	902	31/31	0.95	0.23	70,99,130,144	0
4	MG	E	904	1/1	0.95	0.33	100,100,100,100	0
3	AGS	C	903	31/31	0.96	0.21	79,114,143,164	0
3	AGS	D	902	31/31	0.96	0.18	79,106,154,239	0
4	MG	D	904	1/1	0.96	0.10	139,139,139,139	0
4	MG	B	904	1/1	0.96	0.28	99,99,99,99	0
4	MG	F	904	1/1	0.96	0.29	70,70,70,70	0
3	AGS	B	901	31/31	0.96	0.24	63,101,152,169	0
3	AGS	D	903	31/31	0.96	0.23	66,97,120,134	0
4	MG	E	903	1/1	0.96	0.11	115,115,115,115	0
3	AGS	C	902	31/31	0.96	0.30	72,100,145,218	0
3	AGS	E	901	31/31	0.96	0.18	81,106,140,164	0
3	AGS	A	901	31/31	0.96	0.29	71,108,176,255	0
3	AGS	A	902	31/31	0.96	0.24	55,100,134,142	0
4	MG	F	903	1/1	0.97	0.19	199,199,199,199	0
4	MG	C	905	1/1	0.97	0.25	102,102,102,102	0
4	MG	A	904	1/1	0.98	0.29	86,86,86,86	0

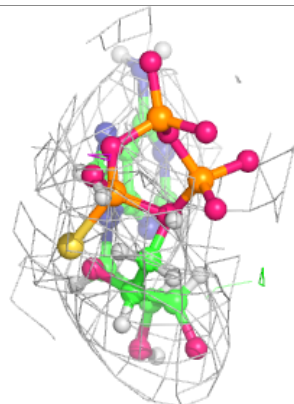
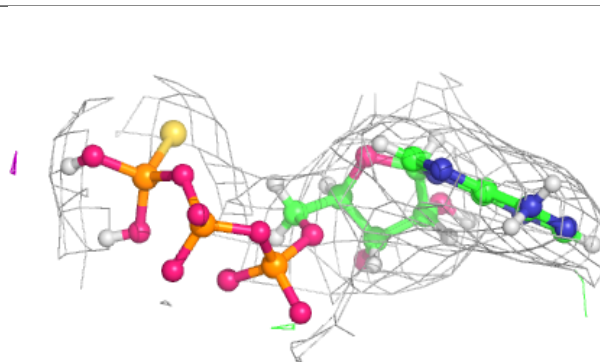
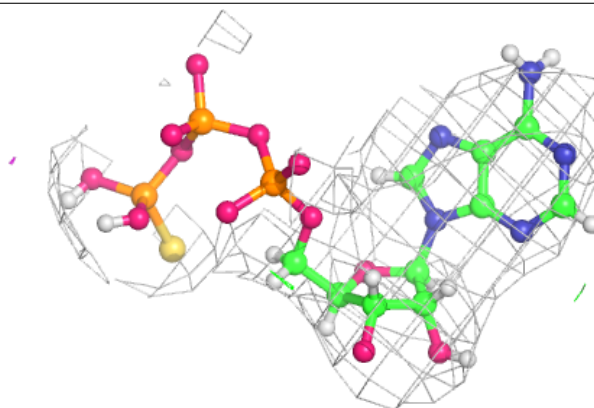
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around AGS 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)

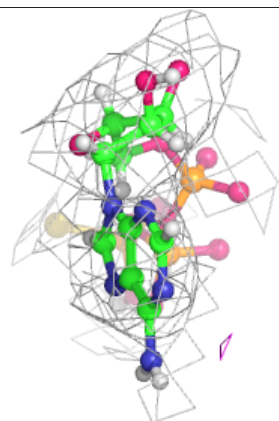
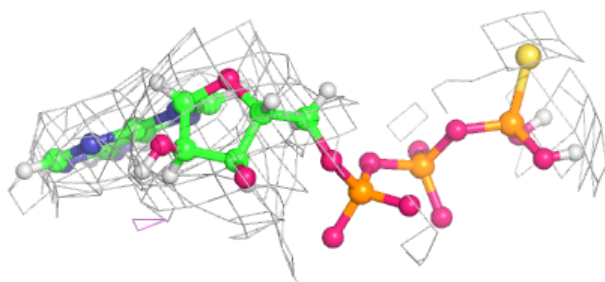
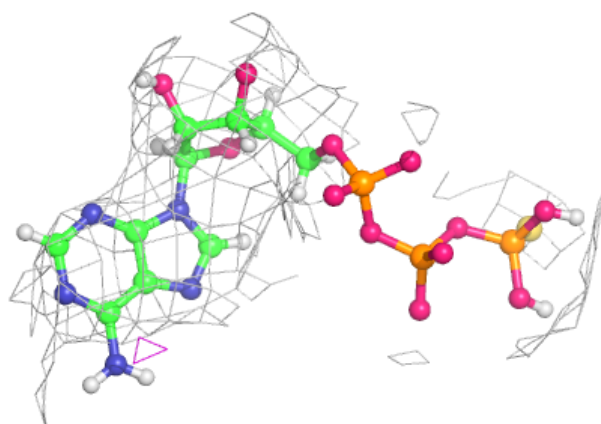
**Electron density around AGS E 902:**

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and green (positive)

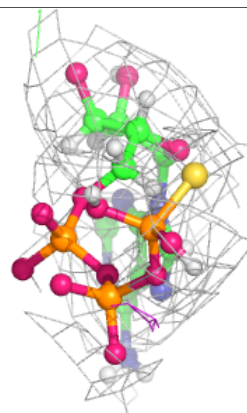
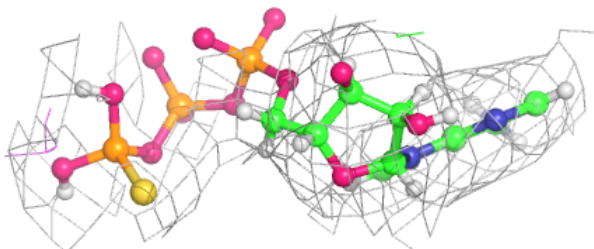
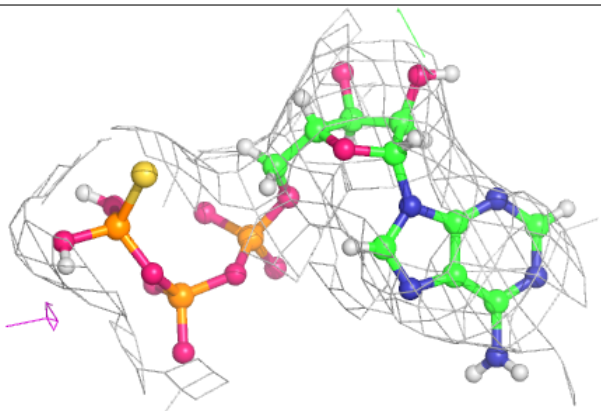


**Electron density around AGS F 901:**

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

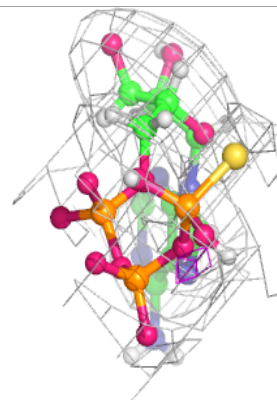
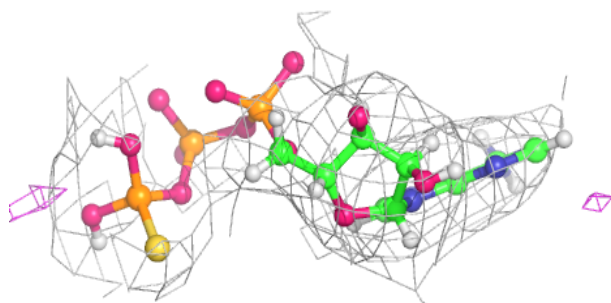
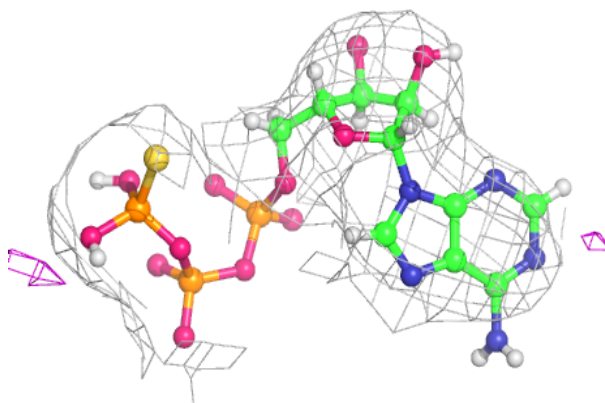
**Electron density around AGS B 902:**

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

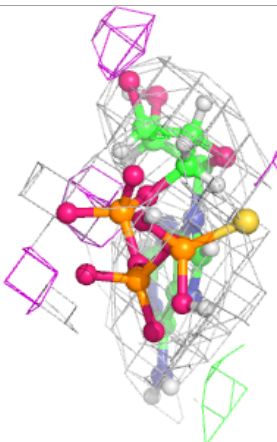
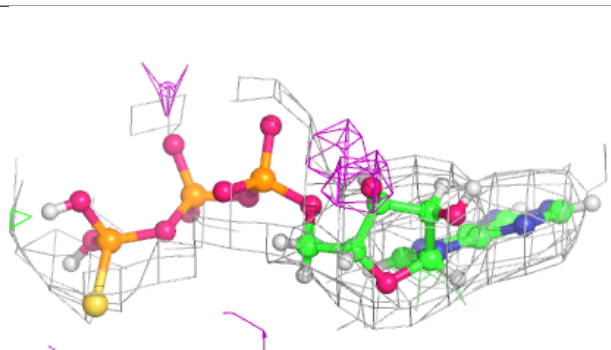
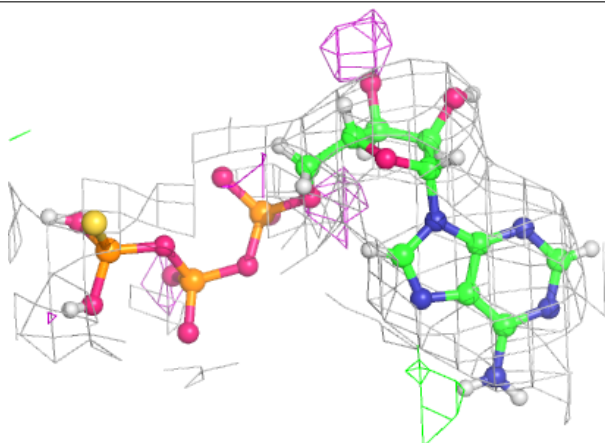


**Electron density around AGS C 903:**

$2mF_o-DF_c$  (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:**

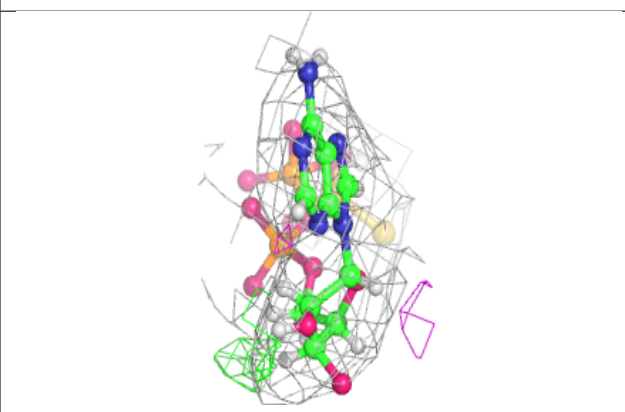
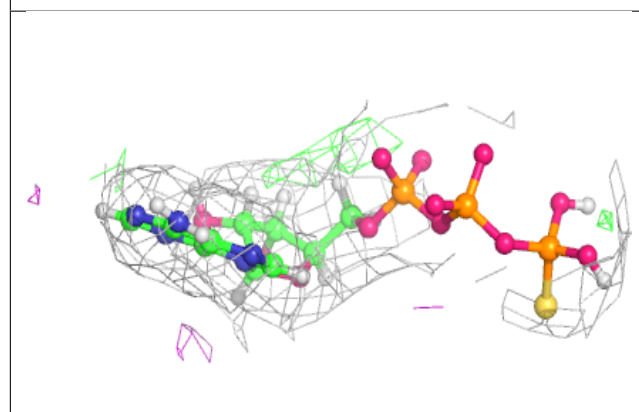
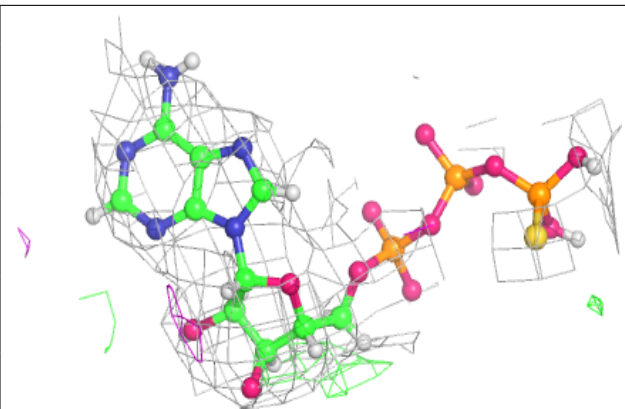
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



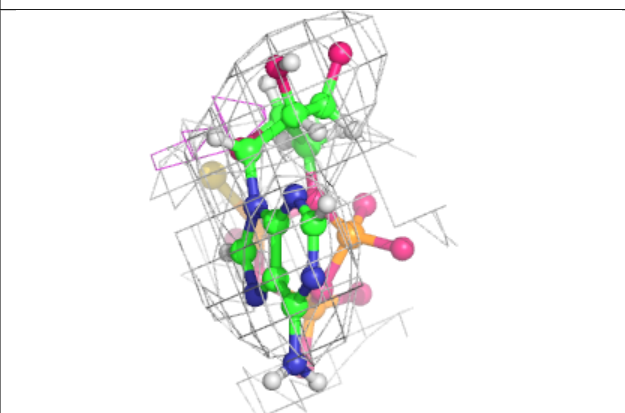
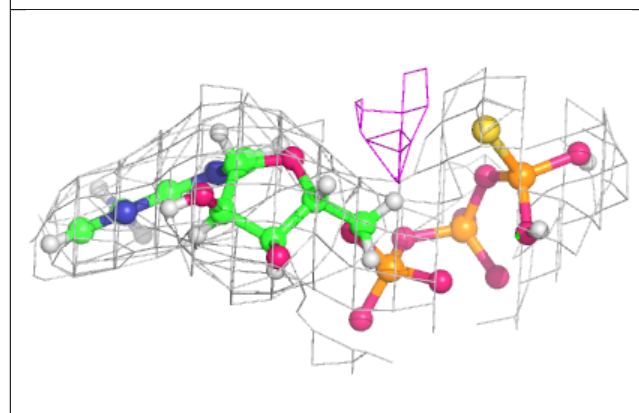
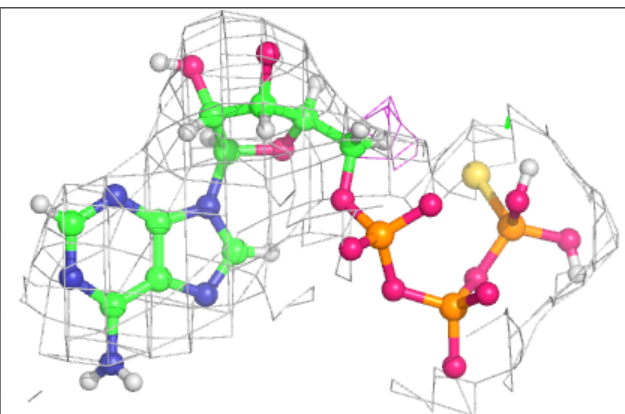


**Electron density around AGS B 901:**

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

**Electron density around AGS D 903:**

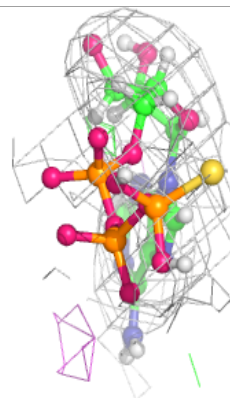
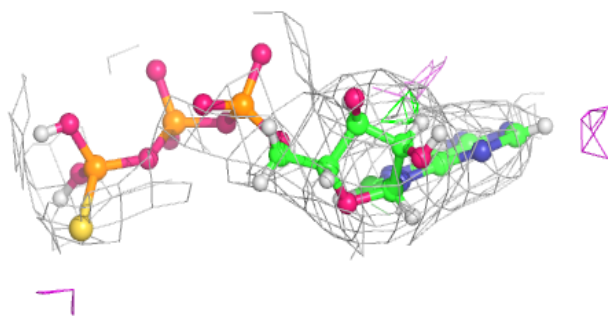
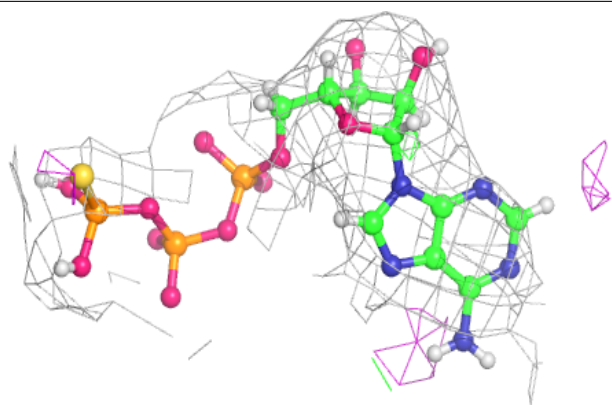
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



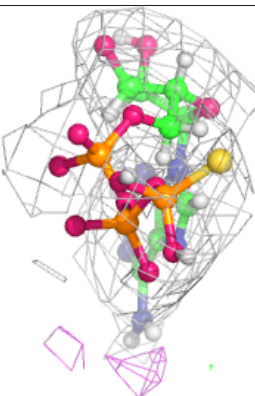
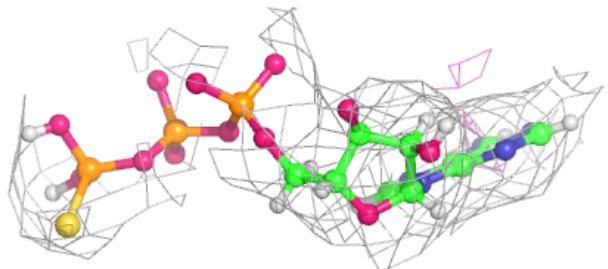
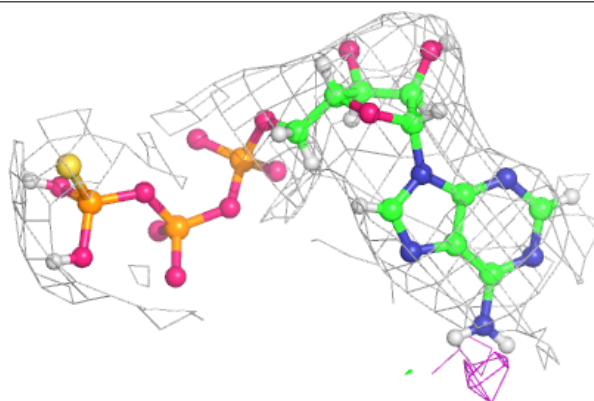


**Electron density around AGS C 902:**

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

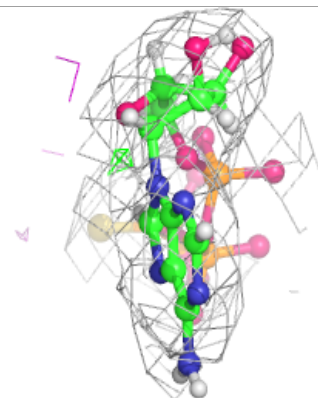
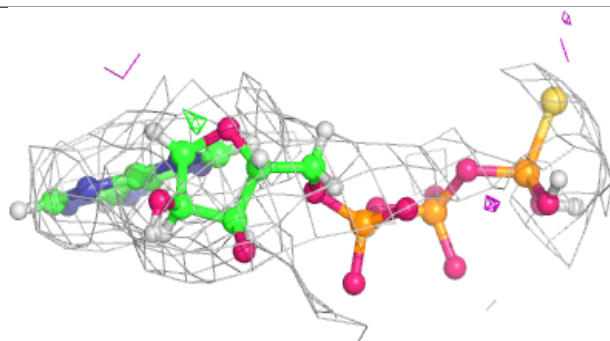
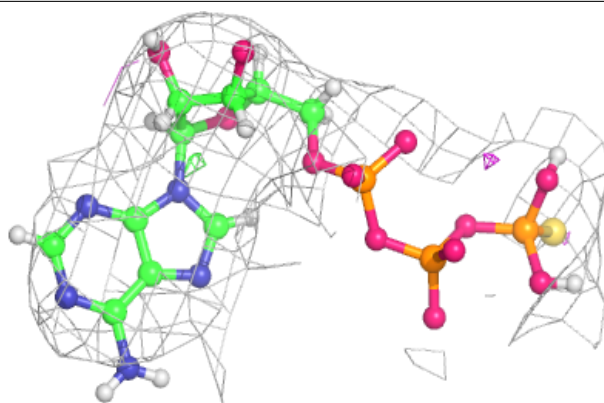
**Electron density around AGS E 901:**

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

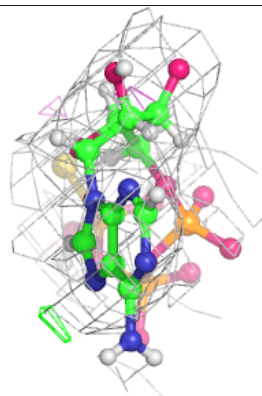
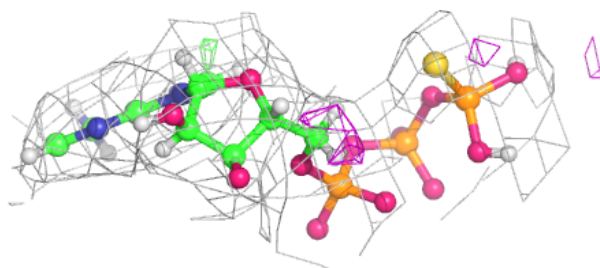
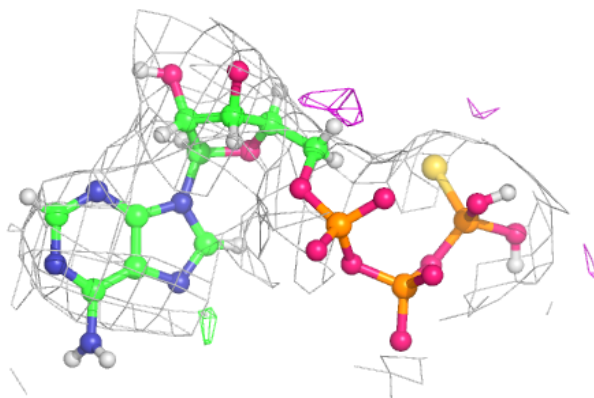


**Electron density around AGS A 901:**

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

**Electron density around AGS 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.