



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 01:59 pm BST

PDB ID : 6KR3  
Title : Crystal structure of Dengue virus nonstructural protein NS5 (form 2)  
Authors : Wu, J.; Lu, G.; Ye, H.Q.; Gong, P.  
Deposited on : 2019-08-20  
Resolution : 2.93 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	:	2.11
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

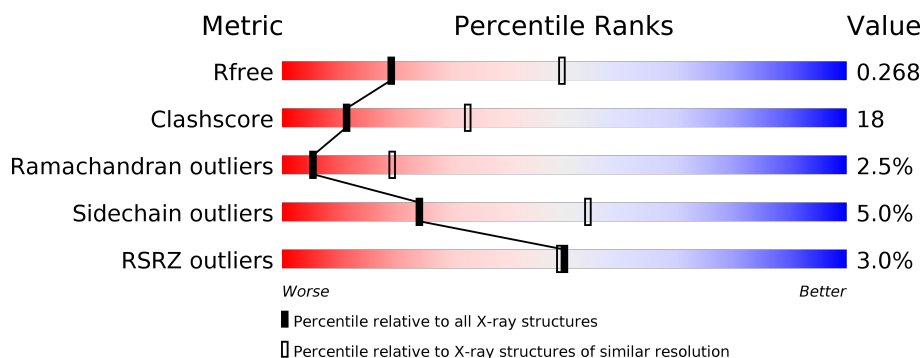
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.93 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	911	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 61%, yellow 28%, orange 1%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>%</span> <span>61%</span> <span>28%</span> <span>• 8%</span> </div> </div>
1	B	911	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, green 58%, yellow 31%, orange 1%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> <span>5%</span> <span>58%</span> <span>31%</span> <span>• 8%</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	B	1009	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12957 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 Genome polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	842	Total	C	N	O	S	0	0	0
			6452	4064	1149	1197	42			
1	B	836	Total	C	N	O	S	0	0	0
			6305	3968	1123	1170	44			

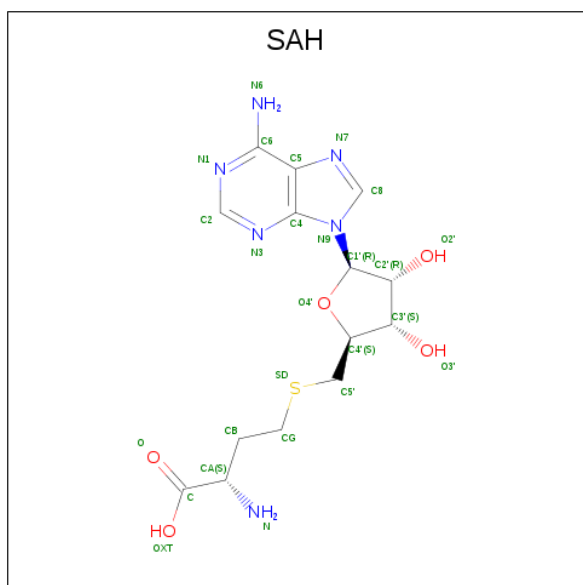
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q91H74
A	901	GLY	-	expression tag	UNP Q91H74
A	902	SER	-	expression tag	UNP Q91H74
A	903	SER	-	expression tag	UNP Q91H74
A	904	SER	-	expression tag	UNP Q91H74
A	905	HIS	-	expression tag	UNP Q91H74
A	906	HIS	-	expression tag	UNP Q91H74
A	907	HIS	-	expression tag	UNP Q91H74
A	908	HIS	-	expression tag	UNP Q91H74
A	909	HIS	-	expression tag	UNP Q91H74
A	910	HIS	-	expression tag	UNP Q91H74
B	0	MET	-	initiating methionine	UNP Q91H74
B	901	GLY	-	expression tag	UNP Q91H74
B	902	SER	-	expression tag	UNP Q91H74
B	903	SER	-	expression tag	UNP Q91H74
B	904	SER	-	expression tag	UNP Q91H74
B	905	HIS	-	expression tag	UNP Q91H74
B	906	HIS	-	expression tag	UNP Q91H74
B	907	HIS	-	expression tag	UNP Q91H74
B	908	HIS	-	expression tag	UNP Q91H74
B	909	HIS	-	expression tag	UNP Q91H74
B	910	HIS	-	expression tag	UNP Q91H74

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total I 3 3	0	0
2	A	12	Total I 12 12	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 26 14 6 5 1	0	0
3	A	1	Total C N O S 26 14 6 5 1	0	0
3	B	1	Total C N O S 26 14 6 5 1	0	0
3	B	1	Total C N O S 26 14 6 5 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Zn 2 2	0	0
4	A	2	Total Zn 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total	O	0	0
			31	31		
6	B	16	Total	O	0	0
			16	16		







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.84Å 209.97Å 157.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.93 49.81 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.81-2.93) 99.9 (49.81-2.93)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.233 , 0.268 0.234 , 0.268	Depositor DCC
$R_{free}$ test set	3164 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.3	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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, ZN, SAH, IOD

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	0.61	9/6601 (0.1%)	0.70	5/8968 (0.1%)
1	B	0.63	14/6453 (0.2%)	0.68	4/8787 (0.0%)
All	All	0.62	23/13054 (0.2%)	0.69	9/17755 (0.1%)

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	ARG	CZ-NH2	-11.11	1.18	1.33
1	B	212	ARG	NE-CZ	-10.86	1.19	1.33
1	A	698	ARG	NE-CZ	-9.75	1.20	1.33
1	A	68	ARG	CZ-NH1	-9.16	1.21	1.33
1	A	698	ARG	CZ-NH1	-9.04	1.21	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	820	GLU	C-N-CA	-6.69	104.97	121.70
1	A	770	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	B	600	GLY	N-CA-C	-5.61	99.08	113.10
1	B	131	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	698	ARG	NE-CZ-NH1	-5.35	117.62	120.30

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	6452	0	5986	214	1
1	B	6305	0	5713	224	0
2	A	12	0	0	2	0
2	B	3	0	0	0	0
3	A	52	0	38	1	0
3	B	52	0	38	5	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	12	0	16	3	0
5	B	18	0	24	5	0
6	A	31	0	0	2	0
6	B	16	0	0	1	0
All	All	12957	0	11815	438	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 18.

The worst 5 of 438 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:57:ARG:NH1	1:A:212:ARG:NH1	1.93	1.16
1:A:57:ARG:HH11	1:A:212:ARG:NH1	1.41	1.16
1:B:165:LEU:HD21	1:B:197:LEU:HD12	1.26	1.14
1:B:238:MET:HE3	1:B:242:ARG:NH1	1.77	0.99
1:B:165:LEU:HD21	1:B:197:LEU:CD1	1.93	0.99

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:A:163:ARG:NH1	1:A:826:ASP:OD2[6_445]	2.11	0.09

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	832/911 (91%)	738 (89%)	81 (10%)	13 (2%)	9	30
1	B	824/911 (90%)	703 (85%)	92 (11%)	29 (4%)	3	13
All	All	1656/1822 (91%)	1441 (87%)	173 (10%)	42 (2%)	5	19

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	597	ASP
1	A	791	SER
1	A	792	ARG
1	B	171	TRP
1	B	214	SER

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	638/790 (81%)	605 (95%)	33 (5%)	23	53
1	B	605/790 (77%)	576 (95%)	29 (5%)	25	56
All	All	1243/1580 (79%)	1181 (95%)	62 (5%)	24	54

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	791	SER

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Mol	Chain	Res	Type
1	B	34	GLN
1	B	700	TRP
1	A	845	GLN
1	B	116	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	622	GLN
1	A	868	ASN
1	B	502	ASN
1	A	575	ASN
1	B	561	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 19 are monoatomic - leaving 9 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
5	GOL	B	1009	-	5,5,5	0.52	0	5,5,5	0.85	0
5	GOL	A	1017	-	5,5,5	0.50	0	5,5,5	0.85	0
5	GOL	B	1010	-	5,5,5	0.57	0	5,5,5	0.40	0
5	GOL	B	1008	-	5,5,5	0.56	0	5,5,5	0.83	0
3	SAH	A	1014	-	21,28,28	1.26	1 (4%)	20,40,40	2.32	8 (40%)
3	SAH	B	1005	-	21,28,28	1.23	2 (9%)	20,40,40	2.23	5 (25%)
3	SAH	A	1013	-	21,28,28	1.24	3 (14%)	20,40,40	2.02	3 (15%)
5	GOL	A	1018	-	5,5,5	0.45	0	5,5,5	0.42	0
3	SAH	B	1004	-	21,28,28	1.45	2 (9%)	20,40,40	2.06	5 (25%)

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
5	GOL	B	1009	-	-	2/4/4/4	-
5	GOL	A	1017	-	-	4/4/4/4	-
5	GOL	B	1010	-	-	4/4/4/4	-
5	GOL	B	1008	-	-	4/4/4/4	-
3	SAH	A	1014	-	-	1/7/31/31	0/3/3/3
3	SAH	B	1005	-	-	3/7/31/31	0/3/3/3
3	SAH	A	1013	-	-	2/7/31/31	0/3/3/3
5	GOL	A	1018	-	-	2/4/4/4	-
3	SAH	B	1004	-	-	5/7/31/31	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1004	SAH	C2-N3	5.22	1.40	1.32
3	A	1014	SAH	C2-N3	3.93	1.38	1.32
3	B	1005	SAH	C2-N3	3.66	1.38	1.32
3	A	1013	SAH	C2-N3	3.31	1.37	1.32
3	B	1005	SAH	C2-N1	3.11	1.39	1.33

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1014	SAH	N3-C2-N1	-6.22	118.96	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1013	SAH	C5'-SD-CG	-5.59	85.50	102.27
3	A	1013	SAH	N3-C2-N1	-5.31	120.38	128.68
3	B	1005	SAH	N3-C2-N1	-5.30	120.40	128.68
3	B	1004	SAH	N3-C2-N1	-4.74	121.27	128.68

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1014	SAH	C-CA-CB-CG
5	A	1018	GOL	O1-C1-C2-C3
5	B	1009	GOL	C1-C2-C3-O3
5	A	1017	GOL	O1-C1-C2-C3
3	A	1013	SAH	C-CA-CB-CG

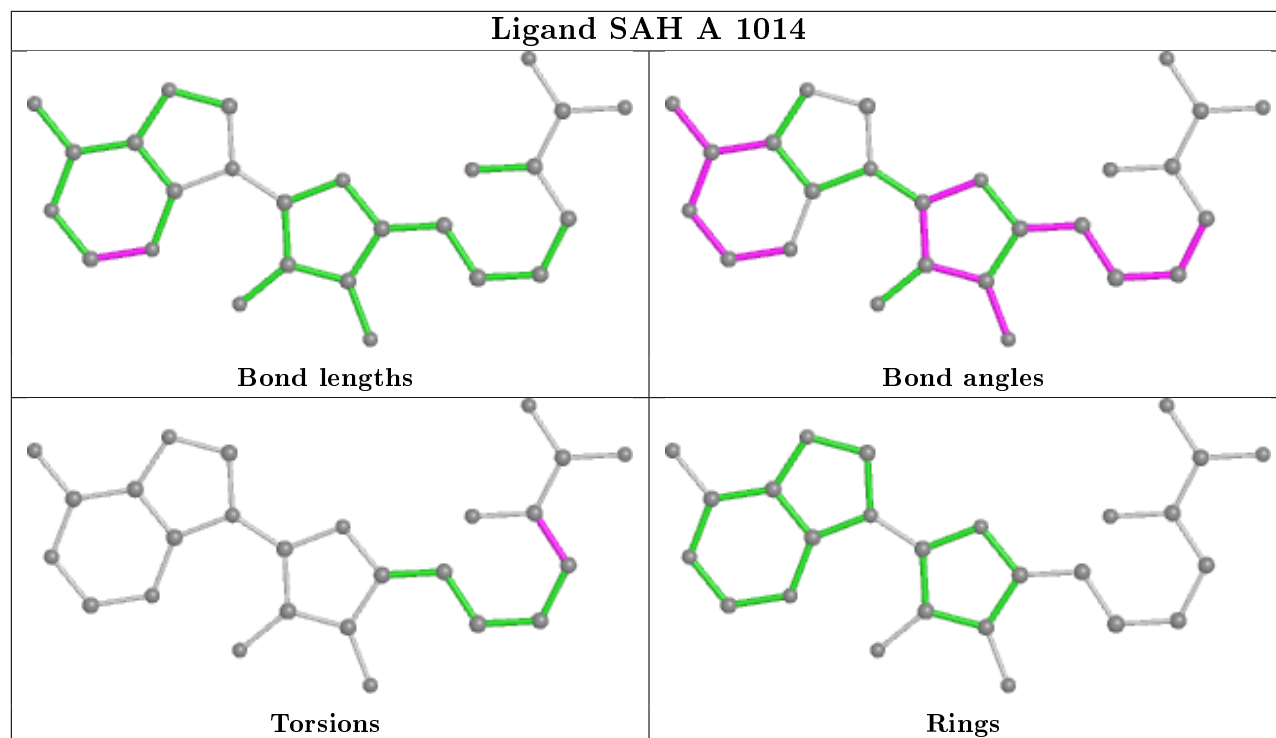
There are no ring outliers.

6 monomers are involved in 14 short contacts:

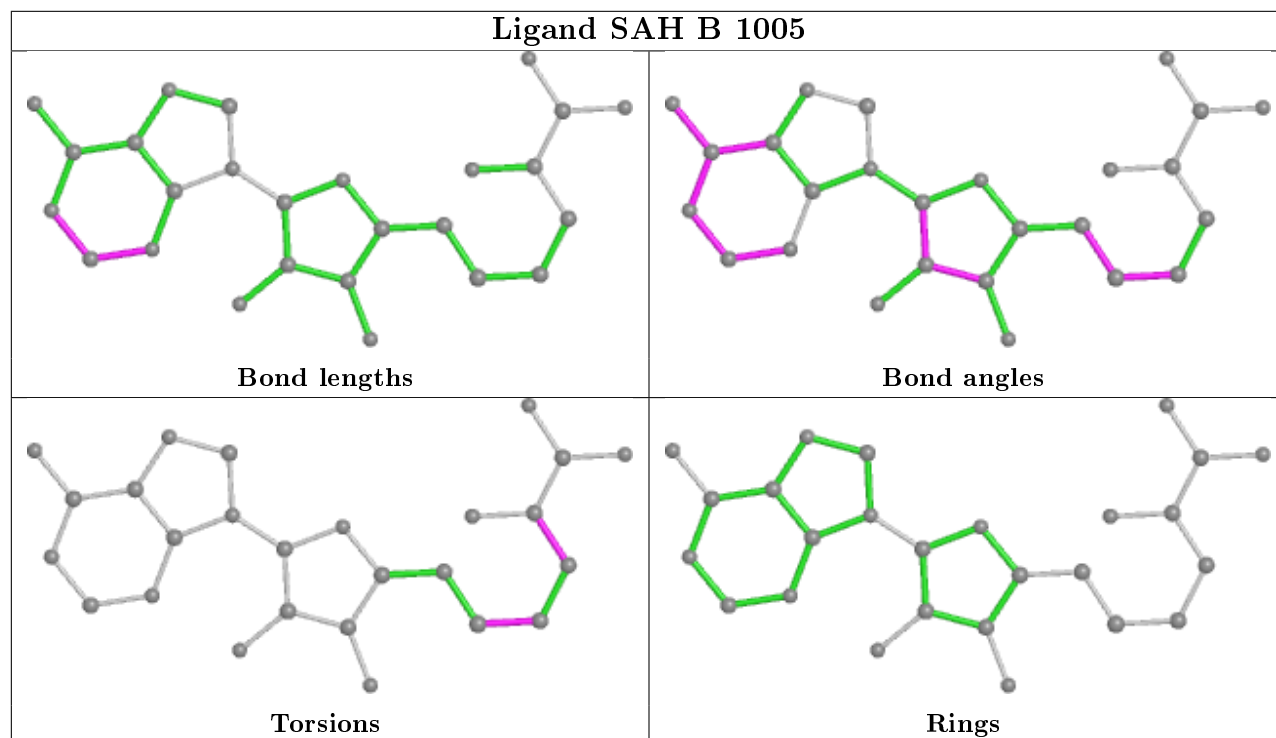
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1009	GOL	5	0
5	A	1017	GOL	2	0
3	B	1005	SAH	4	0
3	A	1013	SAH	1	0
5	A	1018	GOL	1	0
3	B	1004	SAH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

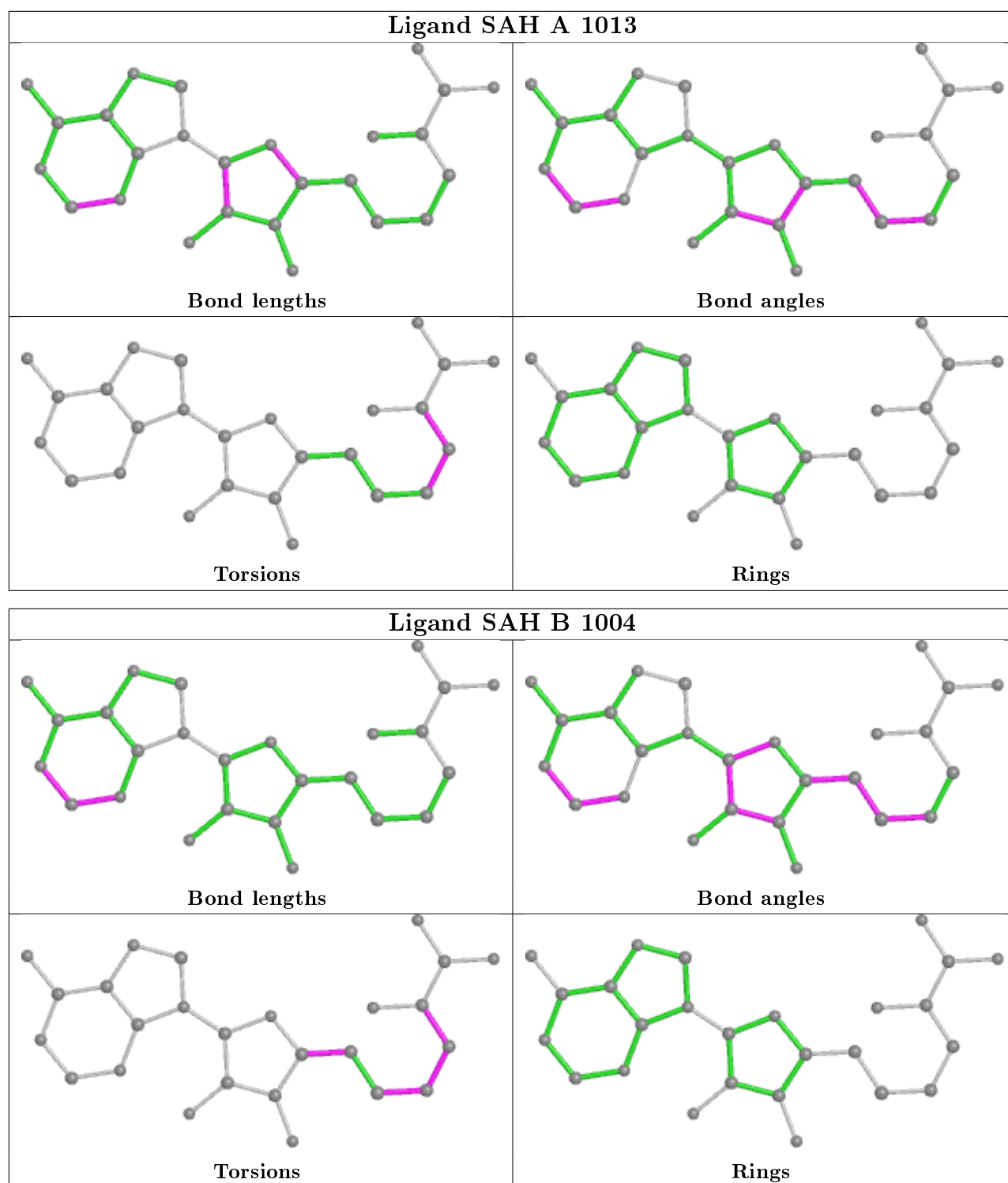
## Ligand SAH A 1014



## Ligand SAH B 1005







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	842/911 (92%)	-0.04	8 (0%) 82 83	33, 51, 78, 97	0
1	B	836/911 (91%)	0.28	42 (5%) 28 28	37, 69, 88, 104	0
All	All	1678/1822 (92%)	0.12	50 (2%) 50 49	33, 59, 85, 104	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	205	LEU	5.6
1	A	795	TRP	5.6
1	A	794	THR	3.6
1	A	313	GLN	3.4
1	B	586	ARG	3.4

### 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 [i](#)

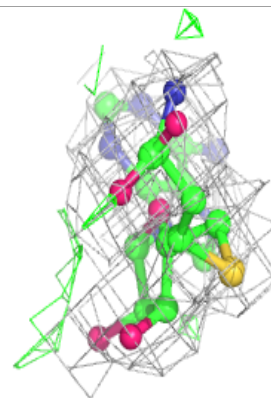
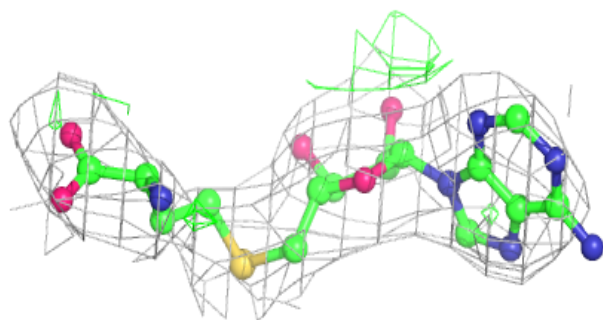
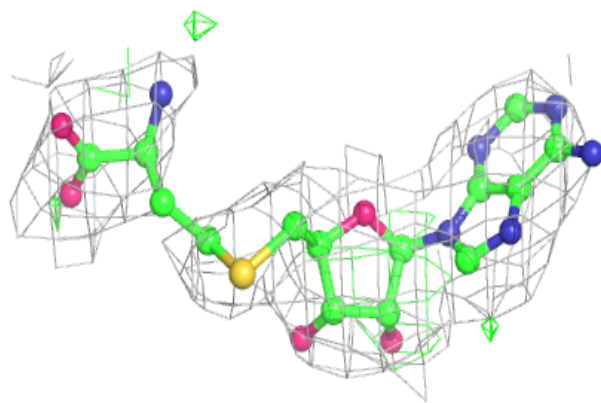
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SAH	B	1005	26/26	0.79	0.23	72,78,84,90	26
3	SAH	B	1004	26/26	0.82	0.21	52,64,74,79	0
3	SAH	A	1014	26/26	0.86	0.21	44,62,73,76	0
4	ZN	B	1006	1/1	0.87	0.13	121,121,121,121	0
5	GOL	A	1017	6/6	0.90	0.21	43,46,48,51	0
5	GOL	B	1010	6/6	0.93	0.25	44,46,48,53	6
2	IOD	B	1003	1/1	0.93	0.18	113,113,113,113	1
5	GOL	A	1018	6/6	0.93	0.22	42,46,48,51	6
4	ZN	A	1015	1/1	0.94	0.10	127,127,127,127	0
5	GOL	B	1008	6/6	0.94	0.20	46,48,50,53	0
2	IOD	B	1002	1/1	0.94	0.08	108,108,108,108	1
2	IOD	A	1008	1/1	0.95	0.20	101,101,101,101	1
2	IOD	A	1012	1/1	0.95	0.16	91,91,91,91	1
3	SAH	A	1013	26/26	0.96	0.20	41,44,54,64	0
2	IOD	A	1003	1/1	0.96	0.12	76,76,76,76	0
2	IOD	A	1007	1/1	0.96	0.07	109,109,109,109	1
2	IOD	A	1006	1/1	0.96	0.14	94,94,94,94	1
2	IOD	B	1001	1/1	0.97	0.07	117,117,117,117	1
2	IOD	A	1011	1/1	0.97	0.08	91,91,91,91	1
5	GOL	B	1009	6/6	0.98	0.13	39,42,43,58	0
4	ZN	A	1016	1/1	0.98	0.14	55,55,55,55	1
2	IOD	A	1009	1/1	0.98	0.11	103,103,103,103	1
4	ZN	B	1007	1/1	0.98	0.13	62,62,62,62	1
2	IOD	A	1010	1/1	0.98	0.07	91,91,91,91	1
2	IOD	A	1002	1/1	0.99	0.17	76,76,76,76	0
2	IOD	A	1005	1/1	0.99	0.12	76,76,76,76	0
2	IOD	A	1001	1/1	1.00	0.11	76,76,76,76	0
2	IOD	A	1004	1/1	1.00	0.27	76,76,76,76	0

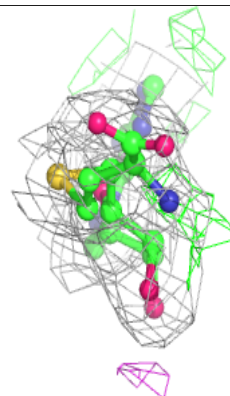
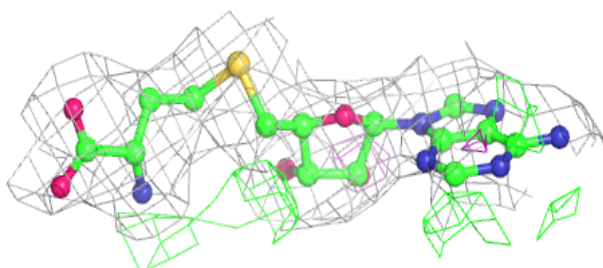
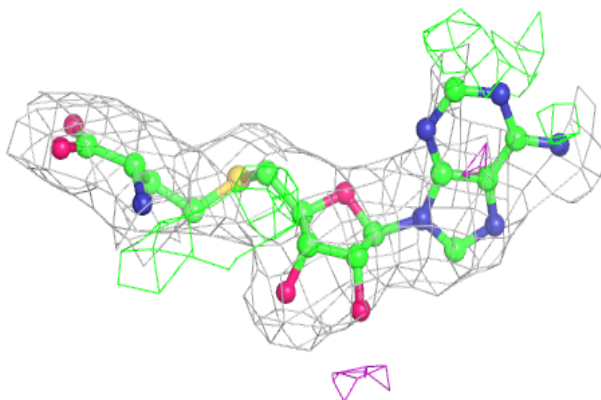
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SAH B 1005:**

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

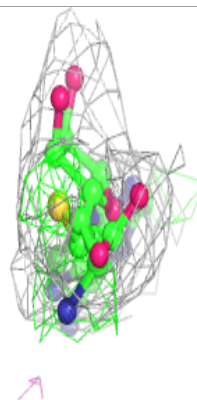
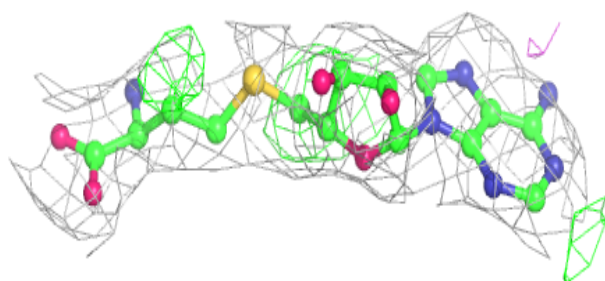
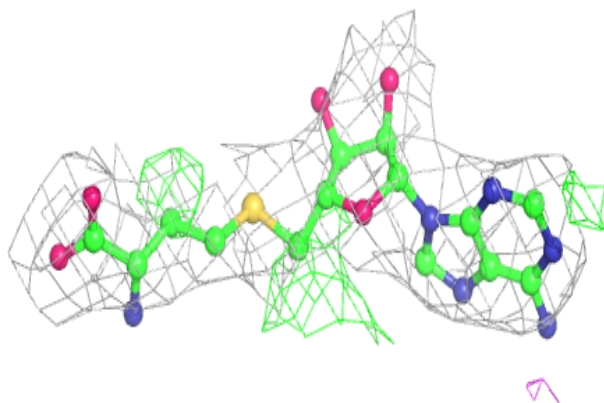
**Electron density around SAH B 1004:**

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



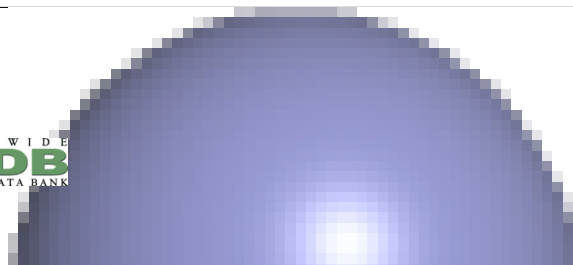
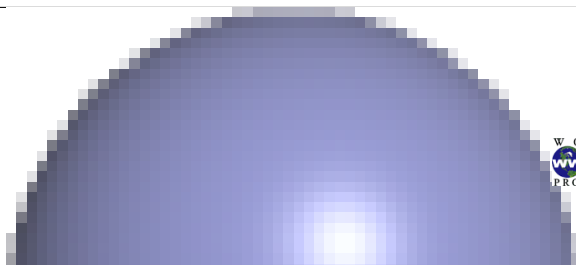
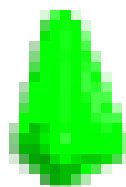
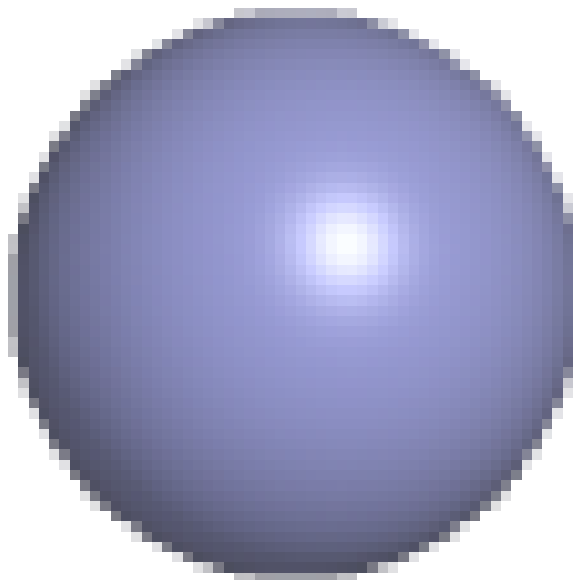
**Electron density around SAH A 1014:**

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



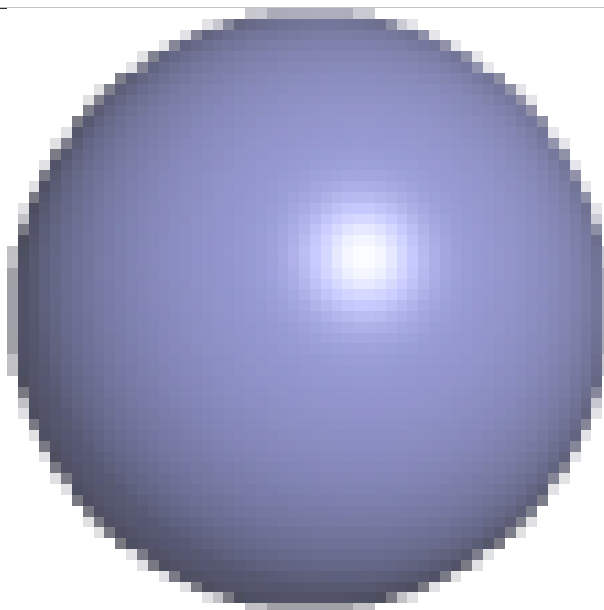
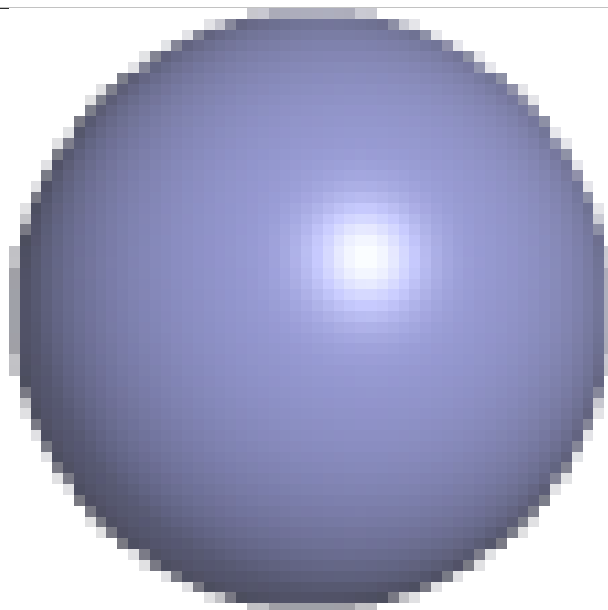
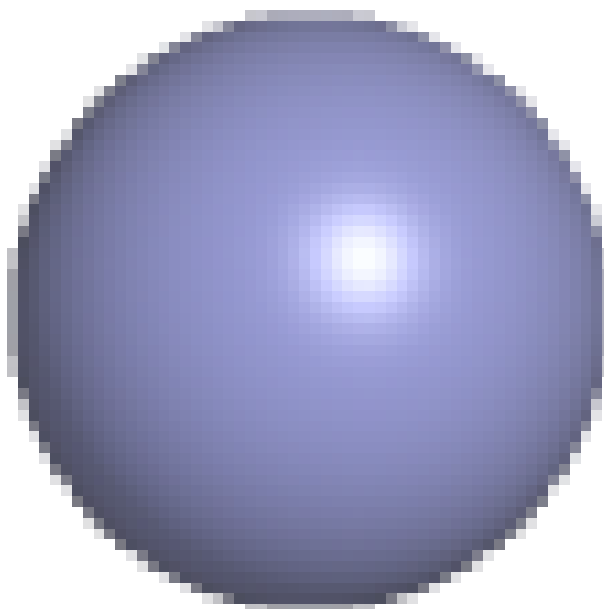
**Electron density around ZN B 1006:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN A 1015:**

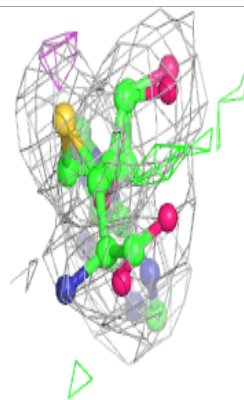
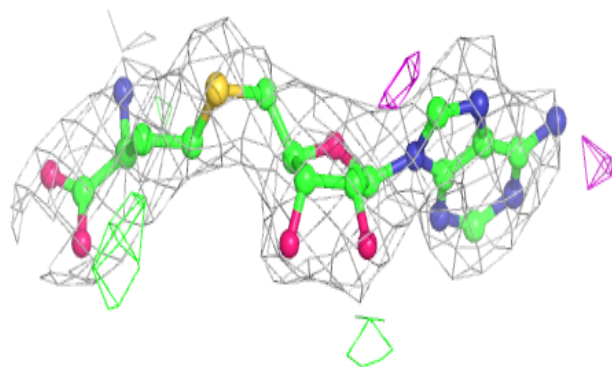
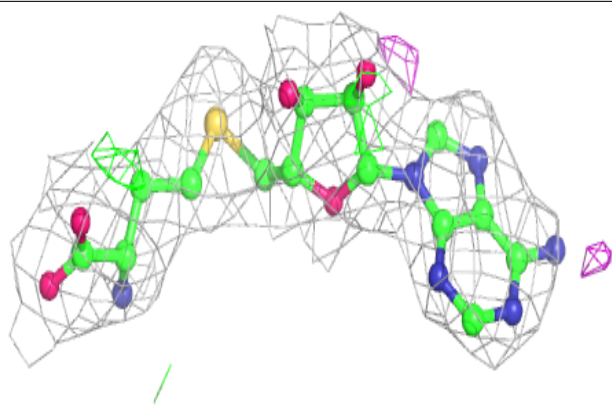
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





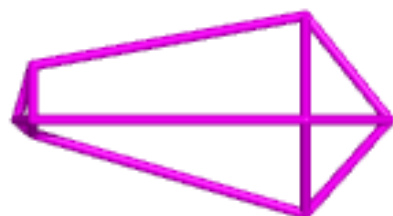
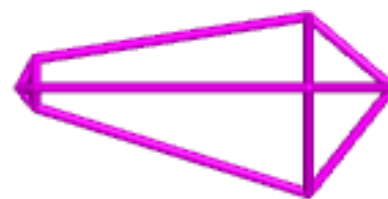
**Electron density around SAH A 1013:**

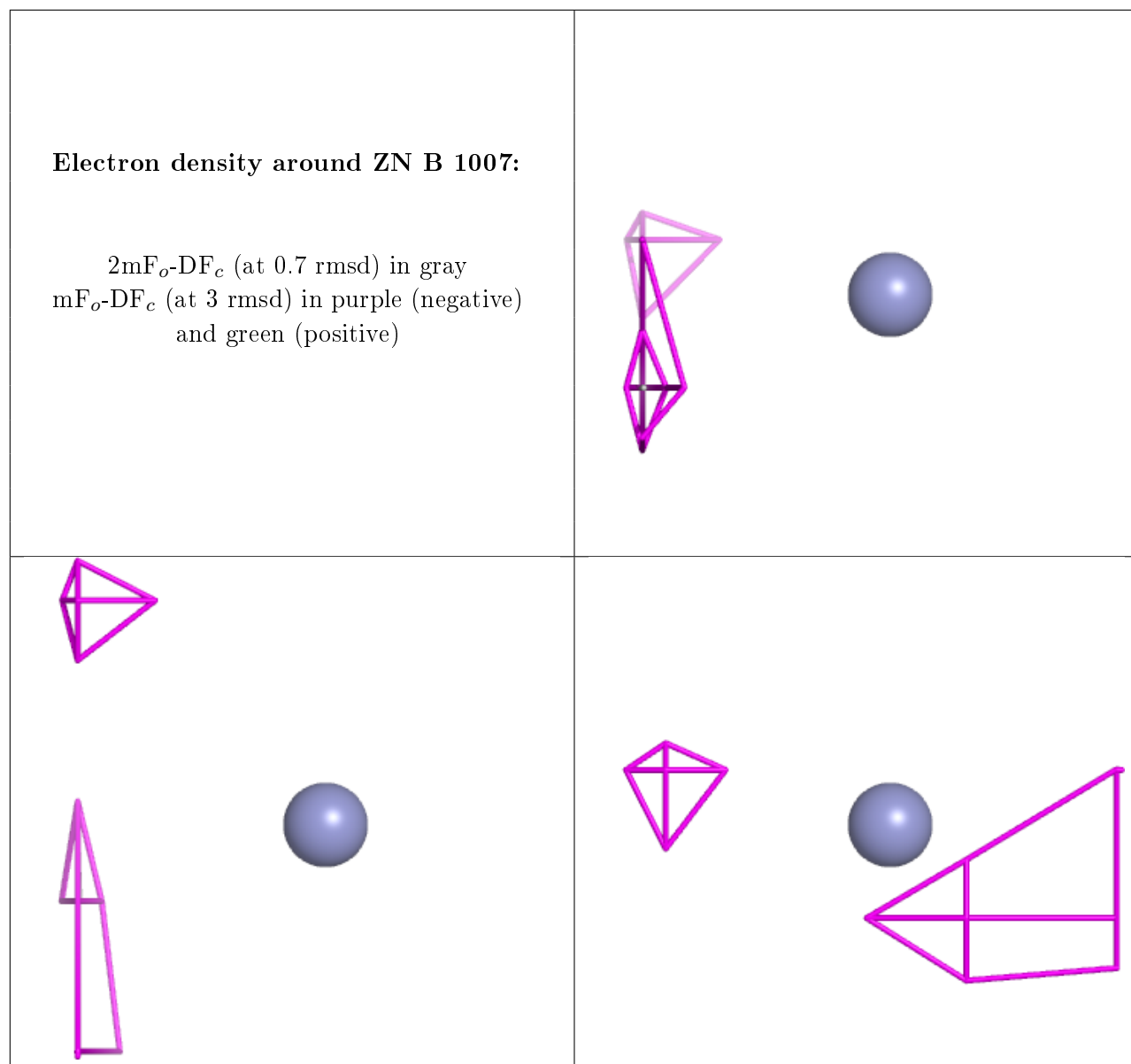
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN A 1016:**

$2mF_o-DF_c$  (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.