



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 05:30 am BST

PDB ID : 6KR2  
Title : Crystal structure of Dengue virus nonstructural protein NS5 (form 1)  
Authors : Wu, J.; Lu, G.; Ye, H.Q.; Gong, P.  
Deposited on : 2019-08-20  
Resolution : 3.06 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

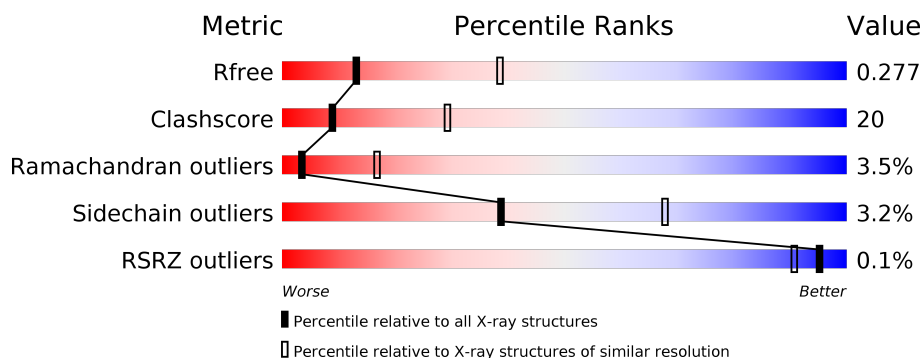
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	
1	B	911	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12727 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	857	Total	C	N	O	S	0	0	0
			6408	4026	1137	1203	42			
1	B	843	Total	C	N	O	S	0	0	0
			6230	3904	1103	1181	42			

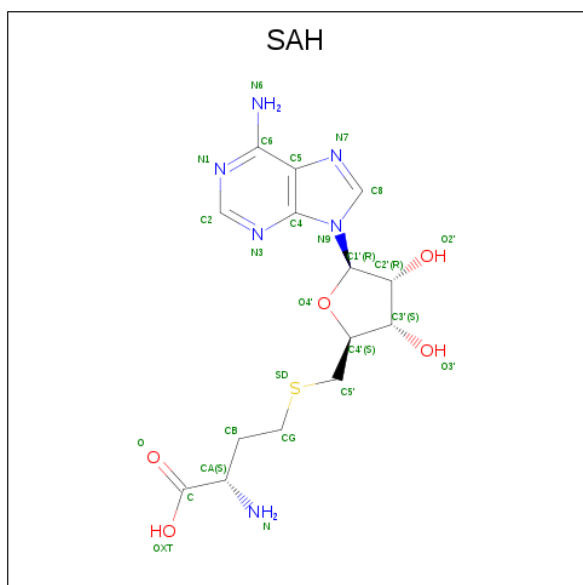
There are 22 discrepancies between the modelled and reference sequences:

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

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

- 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	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

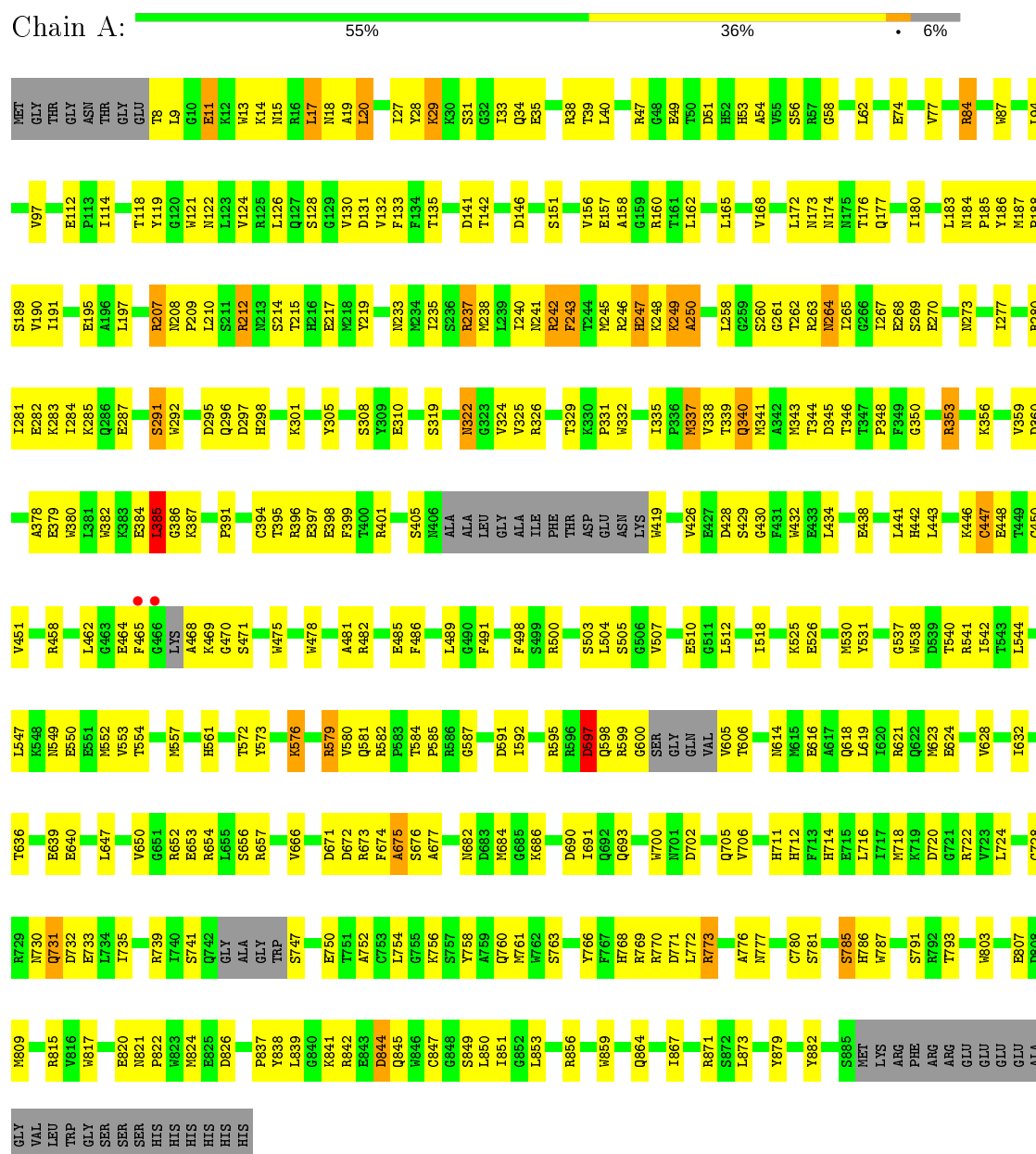
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	15	Total	O	0	0
			15	15		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Genome polypeptide



• Molecule 1: Genome polypeptide

Chain B:  60% 31% 7%

ALA	GLY	VAL	LEU	TRP	GLY	TRP	GLY	THR	ASN	THR	GLY	GLU	T8	L9	G10	E11	K14	N15	R16	L17	N18	A19	L20	F25	Q26	I33	R38	R47	G48	E49	T50	H51	H52	H53	A54	K61	R68	V71	T72	P73	E74	V77	L80	G81	C82	N87	L94	K95	N96	T104	K105
A775	I779	S791	R792	T793	T794	TRP	SER	HIS	HIS	HIS	HIS	HIS	L810	R815	I818	Q819	E820	M824	E825	D826	K827	E831	S832	S833	E834	D844	S849	L850	I851	R856	A857	T858	N862	I863	Q864	L873	M883	PRO	SER	MET	LYS	ARG	PHE	ARG	ARG	GLU	GLU	GLU			
D671	D672	R673	A677	M684	G685	K686	TRP	D690	Q698	S697	W703	V706	P707	F708	C709	S710	E715	E718	R722	V723	L724	W725	V726	R729	N730	Q731	E732	L733	I734	T735	G736	R737	A738	R739	Q742	GLY	ALA	GLY	TRP	S747	Y758	Y766	F767	H768	R769	D771					
K576	R582	D591	I592	R595	R596	D597	Q598	R599	G600	SER	GLY	GLN	VAL	V605	T606	L609	N610	T611	N614	E615	W616	I620	R621	Q622	M623	E624	V628	F629	Q633	H634	L635	N645	W646	L647	V648	R652	E653	R654	L655	S656	R657	N658	A659	I660	S661	P669	L670				
K402	V403	R404	S405	R406	ALA	LEU	GLY	ALA	ILE	PHE	THR	ASP	GLU	ASN	LYS	TRP	LYS	S421	A425	V426	E427	D428	S429	G430	F431	W432	E433	E438	R439	M440	L441	H442	G445	K446	T449	M454	MET	GLY	LYS	R458	E459	L462	G466	K467	A468	LYS	GLY	SER	ARG	ALA	I474
E310	S316	A317	S318	V321	V325	L328	D333	P336	M337	V338	T344	D345	F349	G350	Q351	Q352	R353	V354	F355	K356	E357	R362	E368	K371	K372	L373	A378	E379	N380	L381	W382	K383	L385	K389	M393	C394	T395	R396	E397	E398	F399	T400	R401								
E195	R207	T215	H216	E217	S222	N227	L228	V229	S230	S231	L235	T240	F243	T244	N245	R246	A250	S260	G261	T262	R263	N264	L265	L267	E268	S269	E270	T271	P272	K279	R280	L281	S291	W292	D295	Q296	D297	H298	P299	Y300	K301	T302	G307	S308	Y309						
G106	G107	P108	G109	H110	E111	E112	M116	S117	T118	M121	V124	R125	L126	Q127	S128	D131	V132	F133	D141	T142	L143	L144	S151	P152	N153	D154	T155	V156	E157	R160	T161	L162	R163	V164	V168	L172	Q177	F178	C179	I180	K181	Y186	M187	P188	S189	V190	I191				

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.22Å 146.42Å 98.39Å 90.00° 105.80° 90.00°	Depositor
Resolution (Å)	44.82 – 3.06 44.82 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.3 (44.82-3.06) 97.9 (44.82-3.05)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.10 _2155: ???	Depositor
R, $R_{free}$	0.224 , 0.275 0.226 , 0.277	Depositor DCC
$R_{free}$ test set	2177 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.823	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 41.7	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	0.87	EDS
Total number of atoms	12727	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: ZN, SAH

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	0.57	1/6558 (0.0%)	0.79	5/8932 (0.1%)
1	B	0.53	1/6372 (0.0%)	0.75	5/8683 (0.1%)
All	All	0.55	2/12930 (0.0%)	0.77	10/17615 (0.1%)

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	B	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	CYS	CB-SG	-10.82	1.63	1.82
1	B	389	LYS	C-N	6.33	1.48	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	B	599	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	A	844	ASP	CB-CG-OD1	6.81	124.43	118.30
1	B	20	LEU	CB-CG-CD2	6.30	121.71	111.00
1	A	20	LEU	CA-CB-CG	6.22	129.61	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	268	GLU	Peptide
1	B	279	LYS	Peptide
1	B	350	GLY	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	6408	0	5754	275	0
1	B	6230	0	5502	219	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	26	0	19	4	0
3	B	26	0	19	0	0
4	A	18	0	0	1	0
4	B	15	0	0	0	0
All	All	12727	0	11294	488	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 20.

The worst 5 of 488 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:785:SER:O	1:A:787:TRP:N	1.97	0.97
1:A:14:LYS:NZ	1:A:151:SER:O	1.97	0.96
1:A:233:ASN:O	1:A:237:ARG:HD3	1.70	0.92
1:A:305:TYR:HH	1:A:308:SER:HG	1.15	0.91
1:B:350:GLY:HA2	1:B:353:ARG:HB2	1.57	0.86

There are no symmetry-related clashes.

## 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	847/911 (93%)	698 (82%)	115 (14%)	34 (4%)	3	14
1	B	829/911 (91%)	698 (84%)	107 (13%)	24 (3%)	4	20
All	All	1676/1822 (92%)	1396 (83%)	222 (13%)	58 (4%)	3	17

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	LYS
1	A	250	ALA
1	A	264	ASN
1	A	265	ILE
1	A	267	ILE

### 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	607/790 (77%)	587 (97%)	20 (3%)	38	67
1	B	582/790 (74%)	564 (97%)	18 (3%)	40	68
All	All	1189/1580 (75%)	1151 (97%)	38 (3%)	39	68

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	690	ASP

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Mol	Chain	Res	Type
1	B	26	GLN
1	B	724	LEU
1	A	773	ARG
1	B	61	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	581	GLN
1	B	622	GLN
1	A	864	GLN
1	A	322	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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	SAH	B	1003	-	21,28,28	1.06	2 (9%)	20,40,40	2.23	4 (20%)
3	SAH	A	2003	-	21,28,28	1.20	1 (4%)	20,40,40	1.93	3 (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
3	SAH	B	1003	-	-	2/7/31/31	0/3/3/3
3	SAH	A	2003	-	-	2/7/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2003	SAH	C2-N3	2.94	1.36	1.32
3	B	1003	SAH	C2-N3	2.41	1.36	1.32
3	B	1003	SAH	C2-N1	2.17	1.37	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1003	SAH	N3-C2-N1	-6.55	118.44	128.68
3	A	2003	SAH	C5'-SD-CG	-5.32	86.32	102.27
3	A	2003	SAH	N3-C2-N1	-5.11	120.69	128.68
3	B	1003	SAH	C5'-SD-CG	-4.88	87.63	102.27
3	B	1003	SAH	C1'-N9-C4	-3.45	120.58	126.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

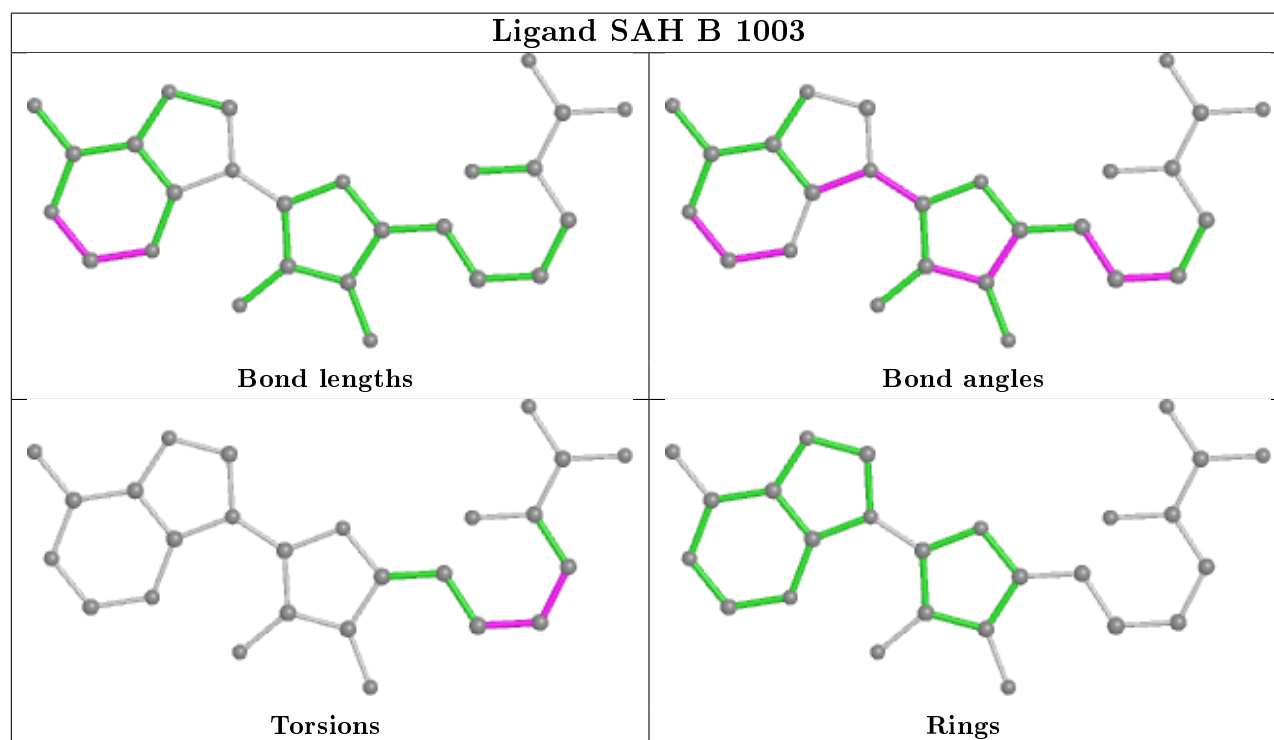
Mol	Chain	Res	Type	Atoms
3	B	1003	SAH	CA-CB-CG-SD
3	A	2003	SAH	CA-CB-CG-SD
3	A	2003	SAH	CB-CG-SD-C5'
3	B	1003	SAH	CB-CG-SD-C5'

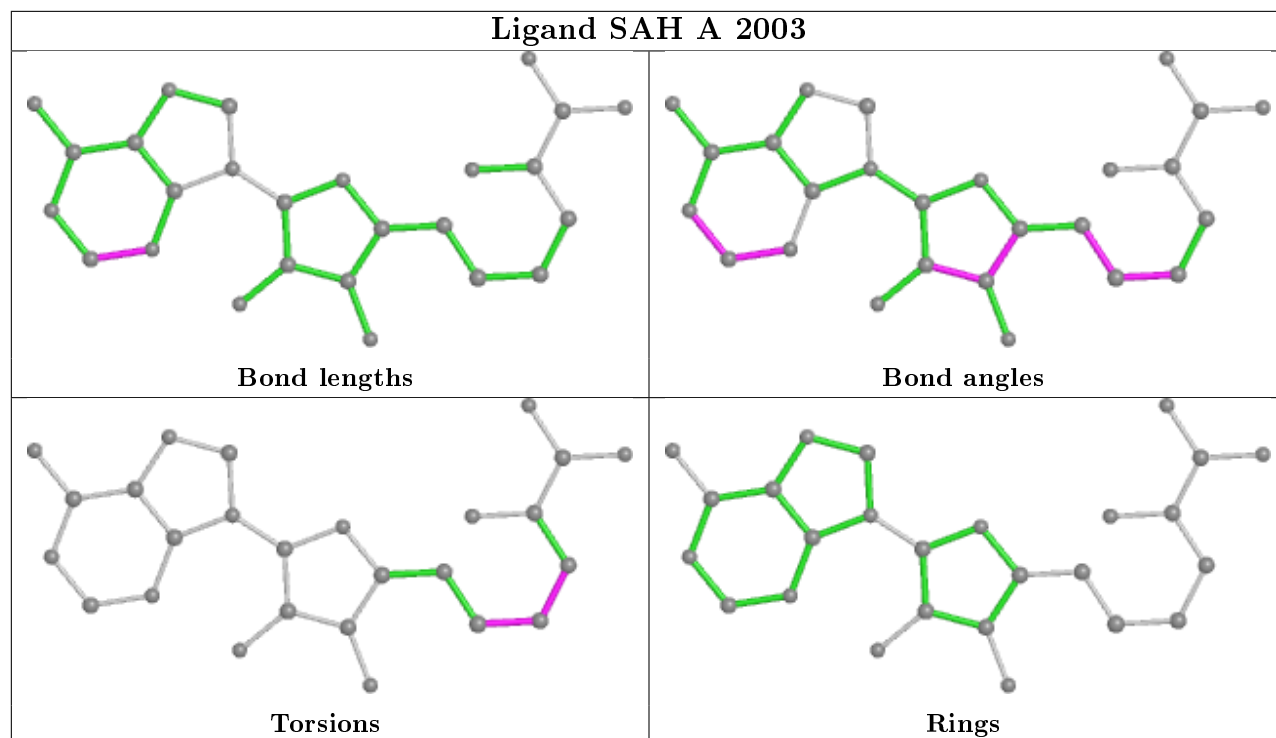
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2003	SAH	4	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	857/911 (94%)	-0.61	2 (0%) 95 89	9, 26, 47, 73	0
1	B	843/911 (92%)	-0.60	0 100 100	11, 27, 50, 87	0
All	All	1700/1822 (93%)	-0.60	2 (0%) 95 91	9, 26, 49, 87	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	PHE	3.5
1	A	466	GLY	2.5

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

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

### 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> )	Q<0.9
2	ZN	A	2001	1/1	0.90	0.29	133,133,133,133	0
3	SAH	B	1003	26/26	0.91	0.24	37,51,57,79	0
3	SAH	A	2003	26/26	0.93	0.24	42,55,62,84	0

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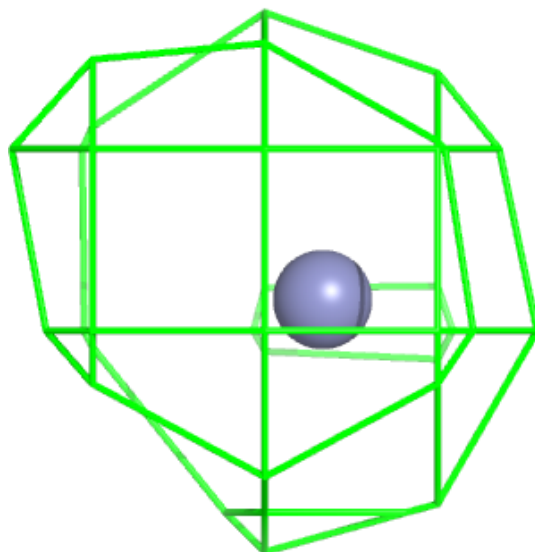
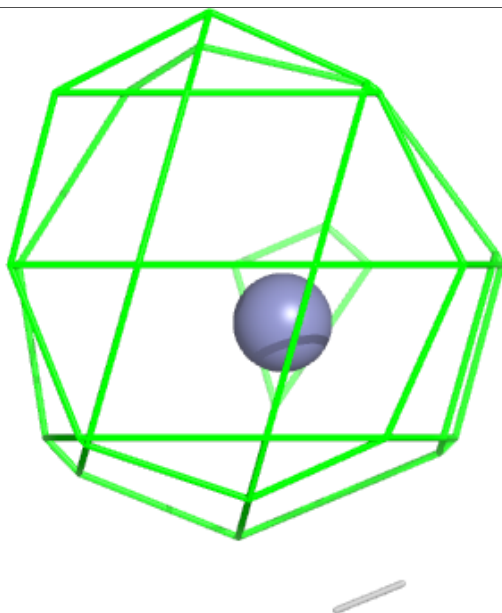
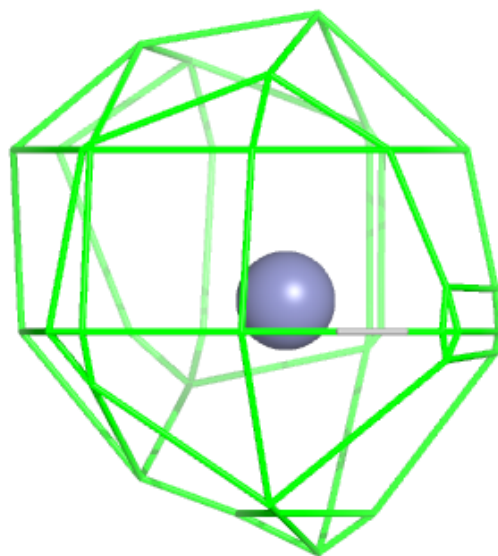
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	2002	1/1	0.94	0.26	128,128,128,128	0
2	ZN	B	1001	1/1	0.99	0.06	23,23,23,23	0
2	ZN	B	1002	1/1	1.00	0.10	20,20,20,20	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 ZN A 2001:**

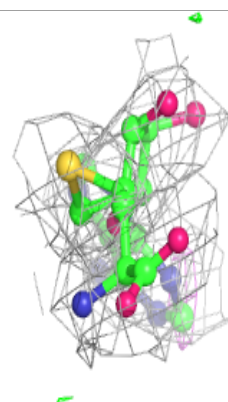
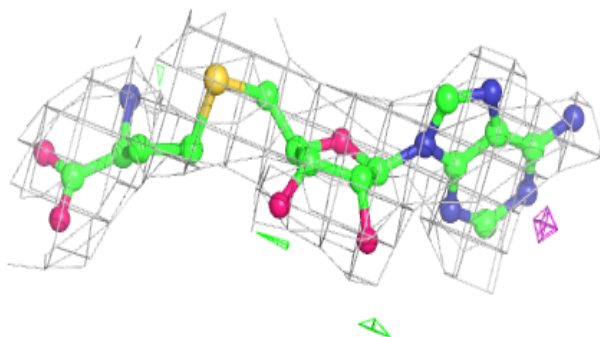
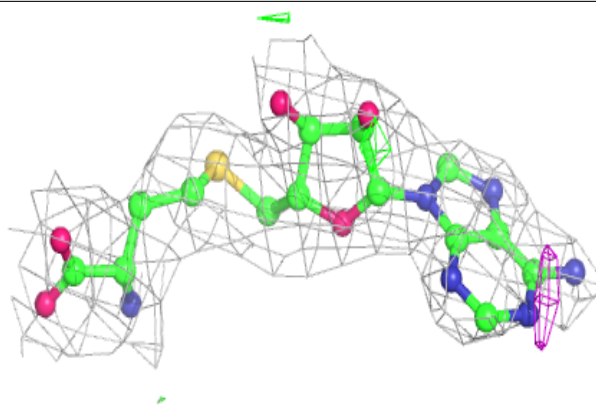
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



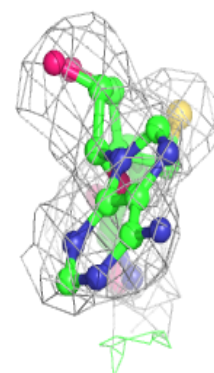
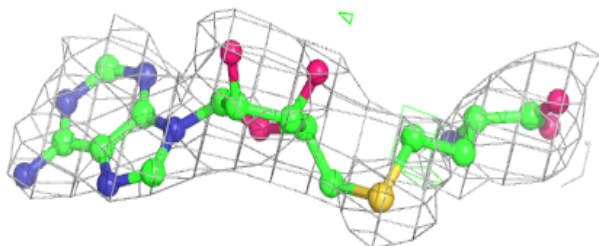
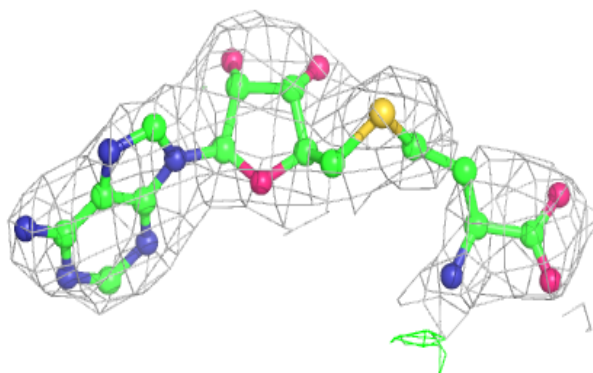


**Electron density around SAH B 1003:**

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

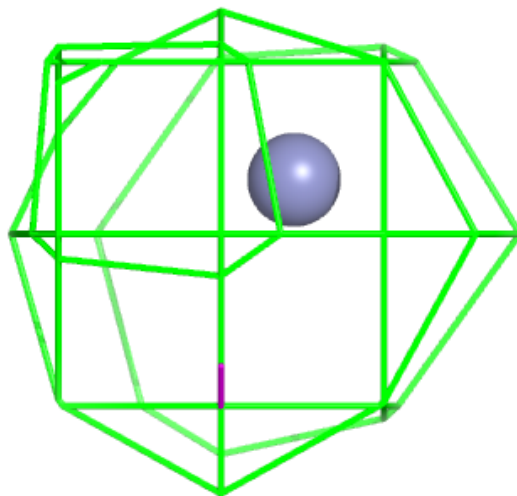
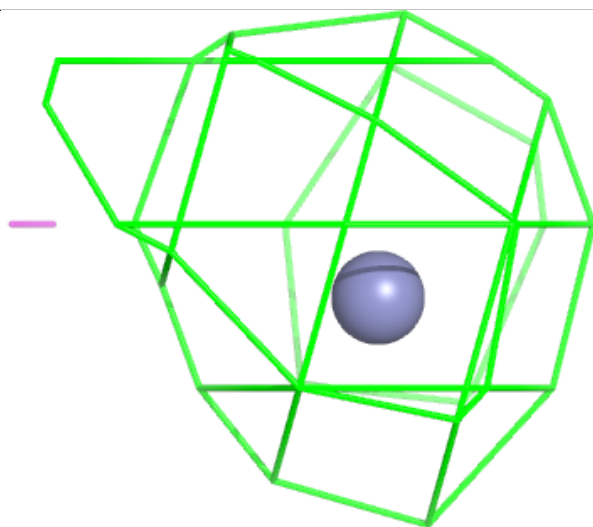
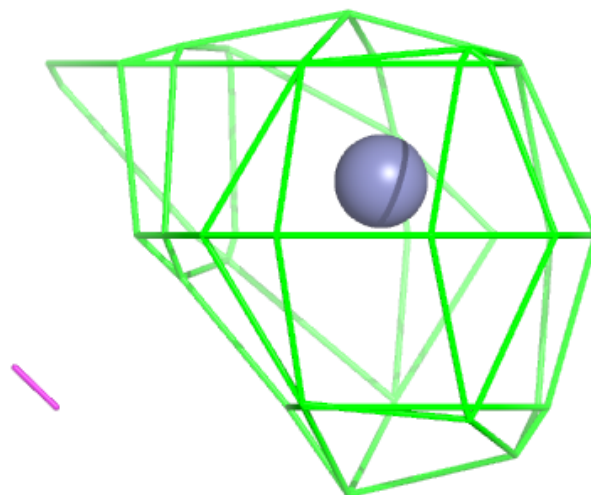
**Electron density around SAH A 2003:**

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



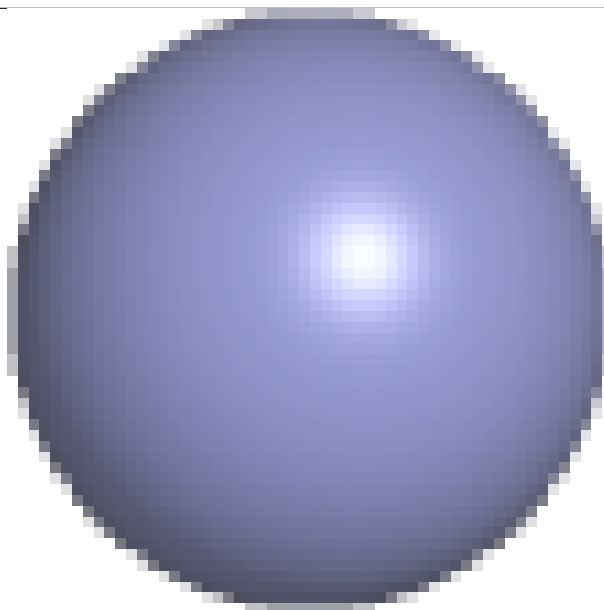
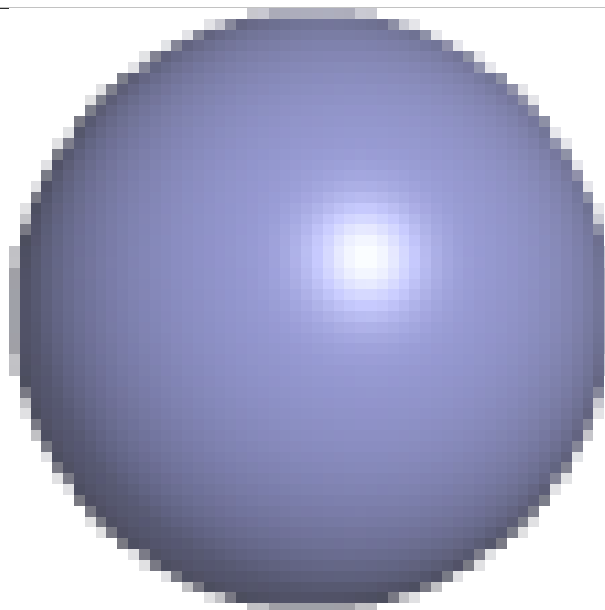
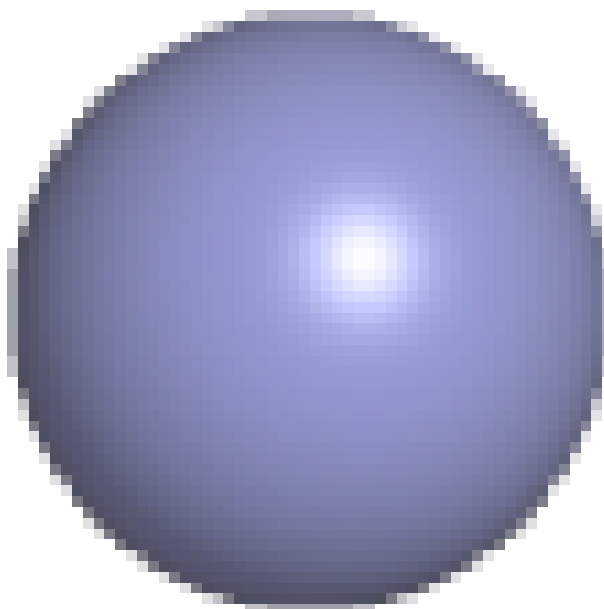
**Electron density around ZN A 2002:**

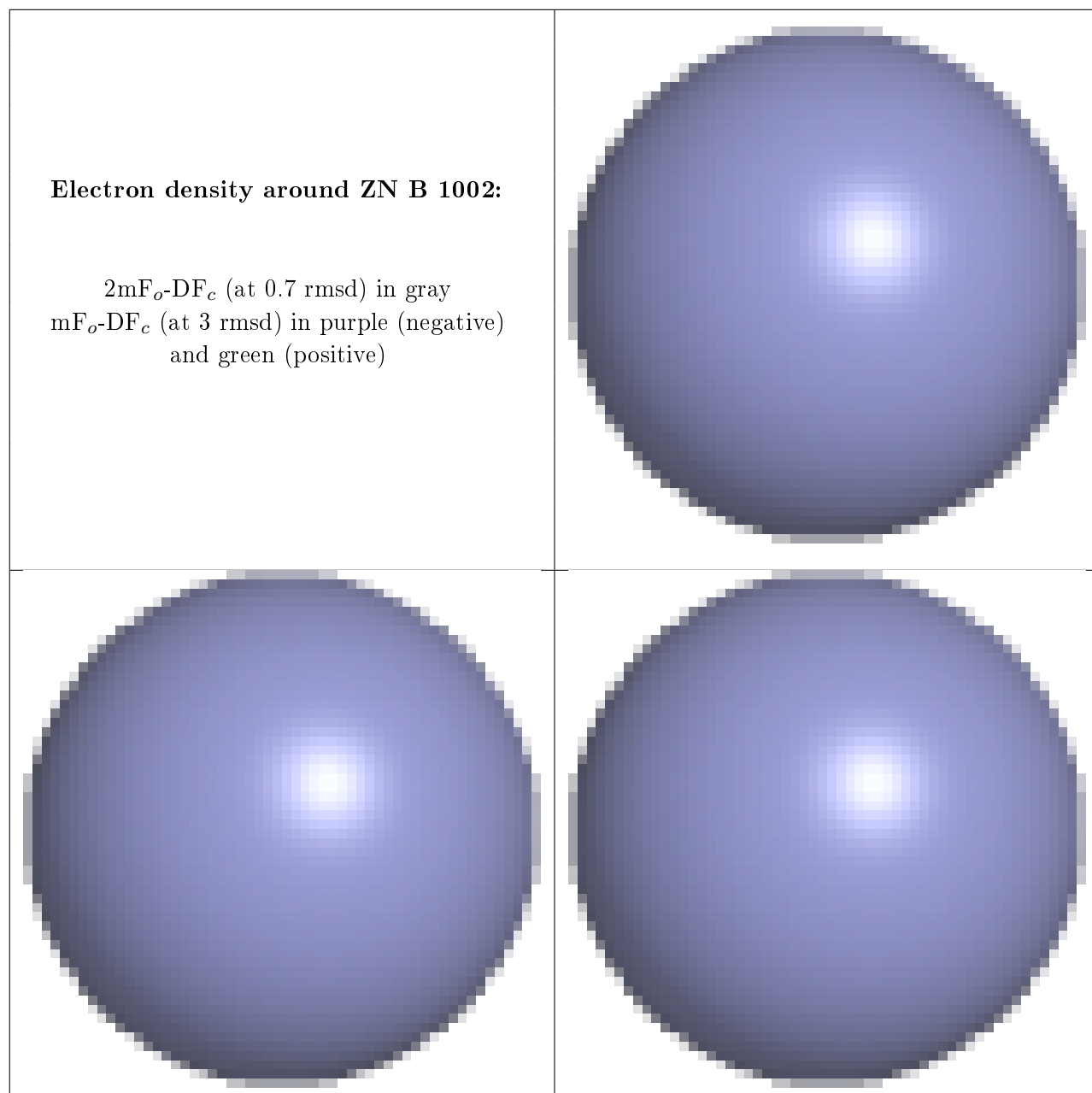
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN B 1001:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.