



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 09:00 am BST

PDB ID : 4XQE  
Title : Crystal Structure of the Homospermidine Synthase (HSS) variant H296S from *Blastochloris viridis* in Complex with NAD and Agmatine  
Authors : Krossa, S.  
Deposited on : 2015-01-19  
Resolution : 1.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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

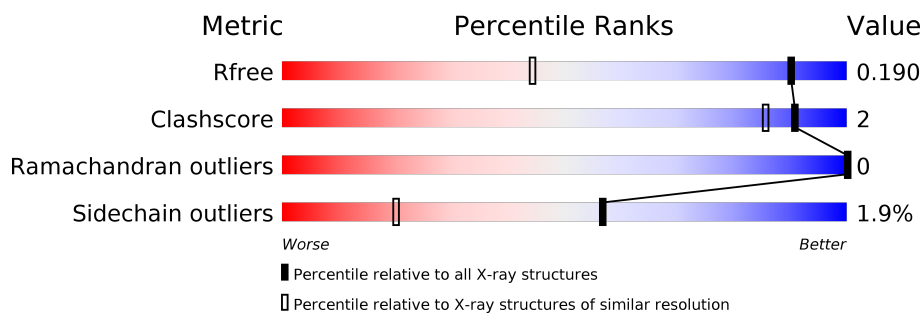
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

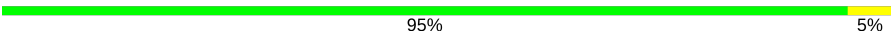

The reported resolution of this entry is 1.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	474	 95% 5%
1	B	474	 96% •

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16526 atoms, of which 7570 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 Homospermidine synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	474	7574	2441	3729	664	722	18	0	21	0
1	B	474	7480	2414	3672	656	721	17	0	15	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	SER	HIS	engineered mutation	UNP O32323
B	296	SER	HIS	engineered mutation	UNP O32323

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	70	21	26	7	14	2	0	0

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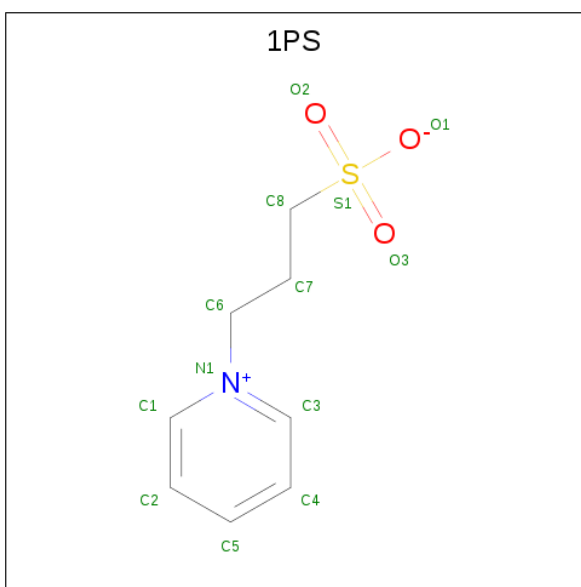
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



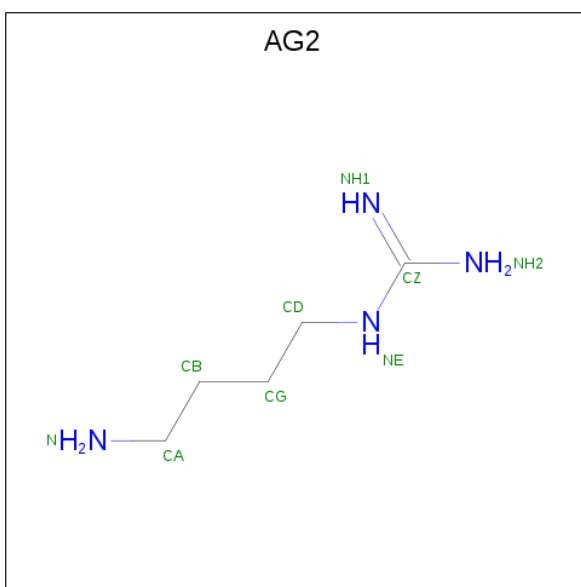
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 3-PYRIDINIUM-1-YLPROPANE-1-SULFONATE (three-letter code: 1PS) (formula: C<sub>8</sub>H<sub>11</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 24	C 8	H 11	N 1	O 3	S 1	0	0
4	A	1	Total 48	C 16	H 22	N 2	O 6	S 2	0	1
4	B	1	Total 48	C 16	H 22	N 2	O 6	S 2	0	1

- Molecule 5 is AGMATINE (three-letter code: AG2) (formula: C<sub>5</sub>H<sub>14</sub>N<sub>4</sub>).



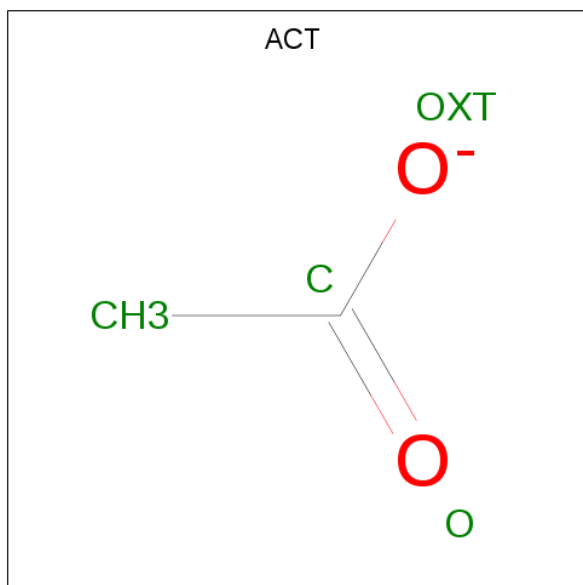
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	N	0	0
			23	5	14	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	N	0	0
			23	5	14	4		
5	B	1	Total	C	H	N	0	0
			23	5	14	4		
5	B	1	Total	C	H	N	0	0
			23	5	14	4		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			7	2	3	2		
6	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	568	Total	O	0	0
			568	568		
7	B	518	Total	O	0	0
			518	518		

### 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. 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. 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: Homospermidine synthase

Chain A: 



- Molecule 1: Homospermidine synthase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.25Å 110.10Å 157.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.30 90.30 – 1.06	Depositor EDS
% Data completeness (in resolution range)	99.1 (10.00-1.30) 71.5 (90.30-1.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.23	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	-0.09 (at 1.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.147 , 0.185 0.153 , 0.190	Depositor DCC
$R_{free}$ test set	22548 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.2	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 46.2	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	0.97	EDS
Total number of atoms	16526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PS, AG2, SO4, NAD, ACT

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	0.45	0/3975	0.63	0/5416
1	B	0.42	0/3916	0.60	0/5338
All	All	0.43	0/7891	0.62	0/10754

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

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	3845	3729	3706	14	0
1	B	3808	3672	3663	9	0
2	A	44	26	22	0	0
2	B	44	26	20	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	39	33	33	5	0
4	B	26	22	22	1	0
5	A	18	28	28	1	0
5	B	18	28	28	0	0
6	A	4	3	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	4	3	3	0	0
7	A	568	0	0	6	2
7	B	518	0	0	8	0
All	All	8956	7570	7528	26	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 2.

The worst 5 of 26 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416[B]:ASN:OD1	7:B:601:HOH:O	1.88	0.89
4:A:507[A]:1PS:O3	7:A:1163:HOH:O	2.00	0.80
1:B:426:ASP:OD1	7:B:956:HOH:O	2.03	0.76
1:B:416[A]:ASN:OD1	7:B:1110:HOH:O	2.08	0.71
1:A:330:ASP:OD1	7:A:1108:HOH:O	2.11	0.67

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)
7:A:686:HOH:O	7:A:697:HOH:O[3_555]	1.91	0.29
7:A:608:HOH:O	7:A:665:HOH:O[3_555]	2.13	0.07

## 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	492/474 (104%)	481 (98%)	11 (2%)	0	100	100
1	B	487/474 (103%)	474 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	979/948 (103%)	955 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	409/388 (105%)	402 (98%)	7 (2%)	60	26
1	B	403/388 (104%)	394 (98%)	9 (2%)	52	15
All	All	812/776 (105%)	796 (98%)	16 (2%)	57	17

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	ASP
1	B	41	LEU
1	B	124[B]	PHE
1	A	323	TYR
1	B	244	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

17 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	502	-	4,4,4	0.22	0	6,6,6	0.09	0
5	AG2	A	506	-	8,8,8	1.94	2 (25%)	7,8,8	0.89	0
2	NAD	A	501	-	42,48,48	4.17	11 (26%)	50,73,73	2.09	12 (24%)
4	1PS	A	507[B]	-	13,13,13	2.14	1 (7%)	17,17,17	1.17	3 (17%)
6	ACT	A	508	-	1,3,3	1.41	0	0,3,3	0.00	-
3	SO4	A	503	-	4,4,4	0.17	0	6,6,6	0.28	0
3	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.21	0
5	AG2	A	505	-	8,8,8	2.00	2 (25%)	7,8,8	1.06	0
3	SO4	A	502	-	4,4,4	0.19	0	6,6,6	0.14	0
2	NAD	B	501	-	42,48,48	4.29	11 (26%)	50,73,73	2.11	9 (18%)
4	1PS	B	506[A]	-	13,13,13	2.08	1 (7%)	17,17,17	1.38	2 (11%)
4	1PS	B	506[B]	-	13,13,13	2.04	1 (7%)	17,17,17	1.65	2 (11%)
6	ACT	B	507	-	1,3,3	1.20	0	0,3,3	0.00	-
5	AG2	B	504	-	8,8,8	1.82	2 (25%)	7,8,8	0.99	0
5	AG2	B	505	-	8,8,8	1.96	2 (25%)	7,8,8	0.77	0
4	1PS	A	504	-	13,13,13	2.10	1 (7%)	17,17,17	1.02	1 (5%)
4	1PS	A	507[A]	-	13,13,13	2.10	1 (7%)	17,17,17	1.51	4 (23%)

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	AG2	A	506	-	-	0/6/6/6	-
2	NAD	A	501	-	-	4/26/62/62	0/5/5/5
4	1PS	A	507[B]	-	-	1/7/7/7	0/1/1/1
5	AG2	A	505	-	-	1/6/6/6	-
2	NAD	B	501	-	-	4/26/62/62	0/5/5/5
4	1PS	B	506[A]	-	-	6/7/7/7	0/1/1/1
4	1PS	B	506[B]	-	-	6/7/7/7	0/1/1/1
5	AG2	B	504	-	-	1/6/6/6	-
5	AG2	B	505	-	-	0/6/6/6	-
4	1PS	A	504	-	-	0/7/7/7	0/1/1/1
4	1PS	A	507[A]	-	-	4/7/7/7	0/1/1/1

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAD	C2D-C1D	-15.60	1.30	1.53
2	A	501	NAD	C2D-C1D	-15.50	1.30	1.53
2	B	501	NAD	O4D-C1D	14.19	1.60	1.41
2	A	501	NAD	O4D-C1D	13.72	1.60	1.41
2	B	501	NAD	C2B-C3B	-10.44	1.24	1.53

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAD	C3D-C2D-C1D	8.30	113.47	100.98
2	A	501	NAD	C3D-C2D-C1D	7.47	112.23	100.98
2	A	501	NAD	C2B-C3B-C4B	6.06	114.41	102.64
2	B	501	NAD	C2B-C3B-C4B	5.18	112.71	102.64
4	B	506[B]	1PS	O3-S1-C8	4.96	112.89	106.92

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

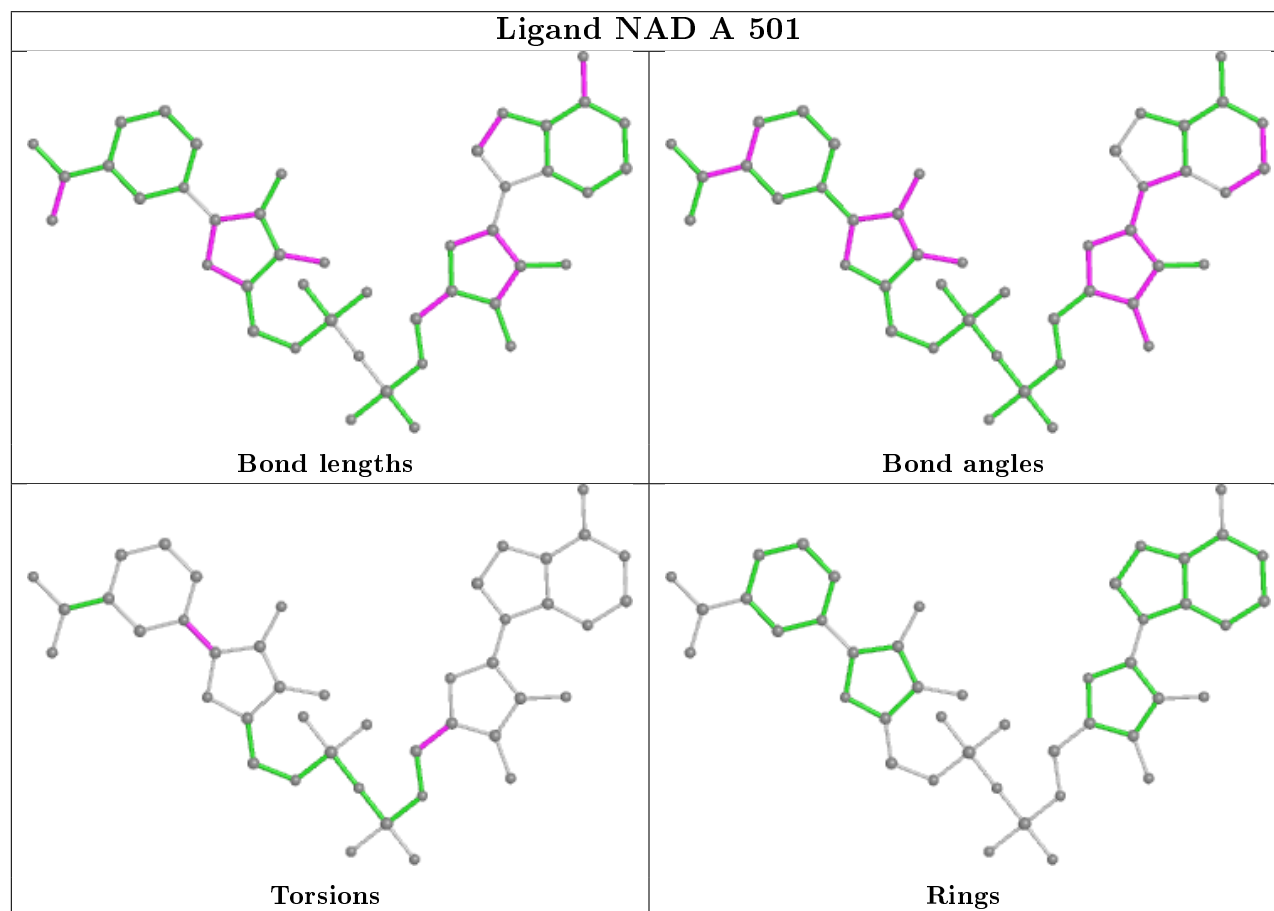
Mol	Chain	Res	Type	Atoms
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
4	A	507[B]	1PS	N1-C6-C7-C8
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N

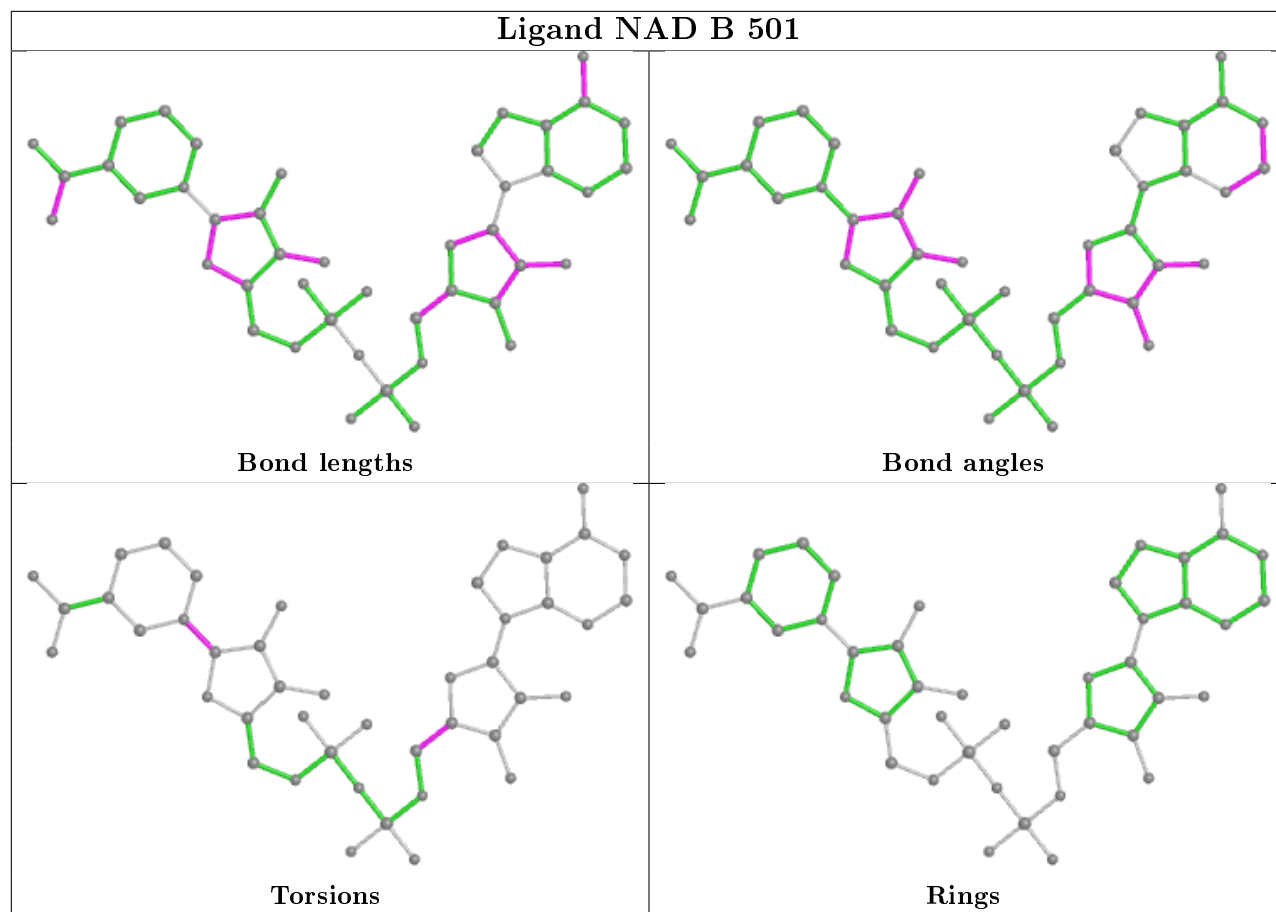
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	507[B]	1PS	2	0
5	A	505	AG2	1	0
4	B	506[B]	1PS	1	0
4	A	507[A]	1PS	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.





## 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

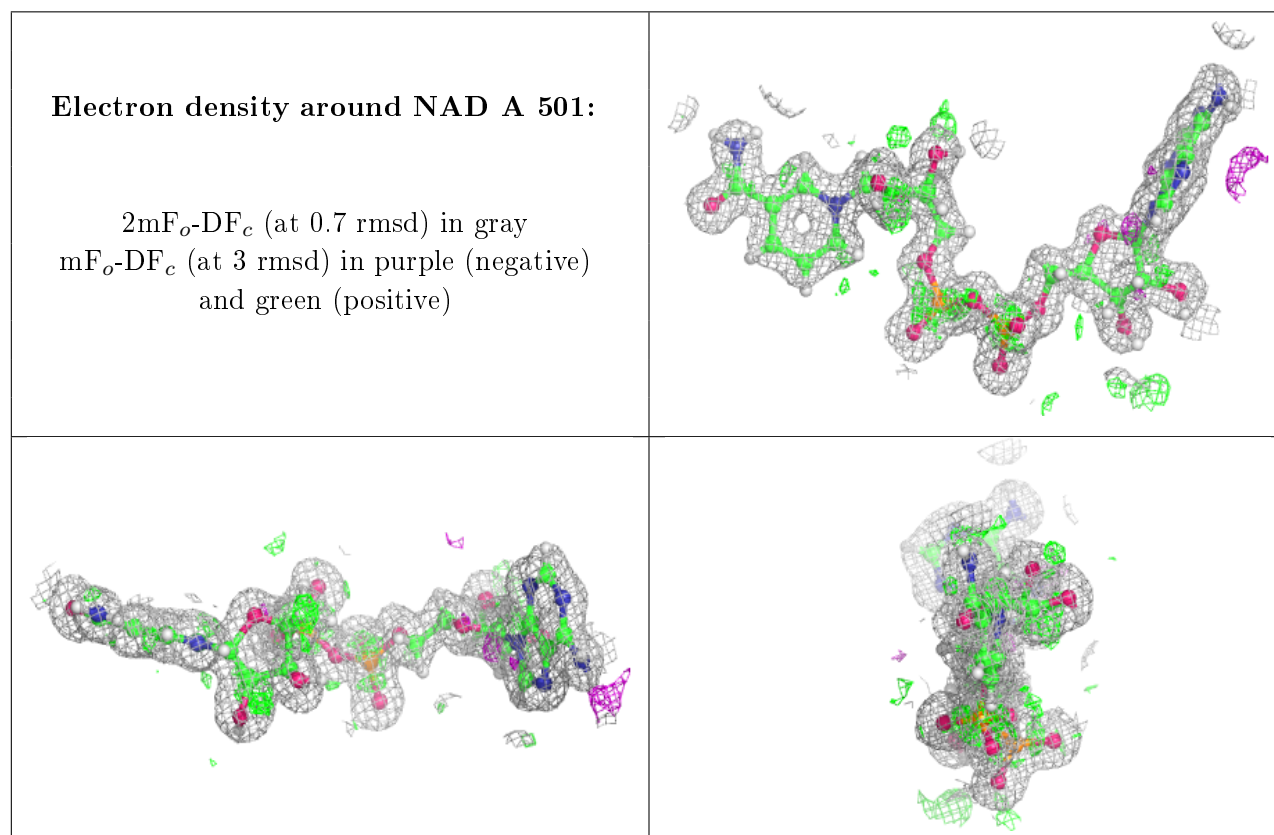
### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

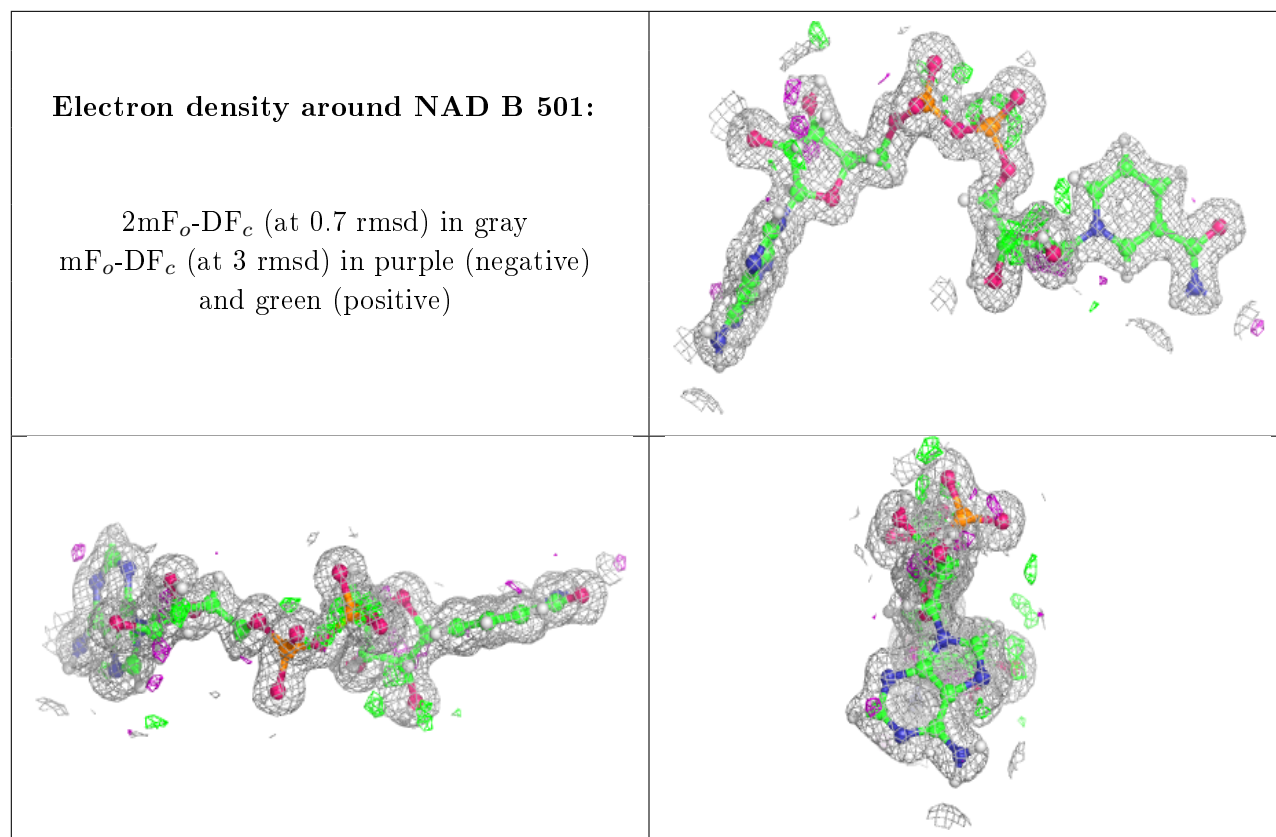
### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.







## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.