



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 06:30 pm GMT

PDB ID : 4XR4
Title : Crystal Structure of the Homospermidine Synthase (HSS) from *Blastochloris viridis* in Complex with NAD and Agmatine
Authors : Krossa, S.
Deposited on : 2015-01-20
Resolution : 1.63 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

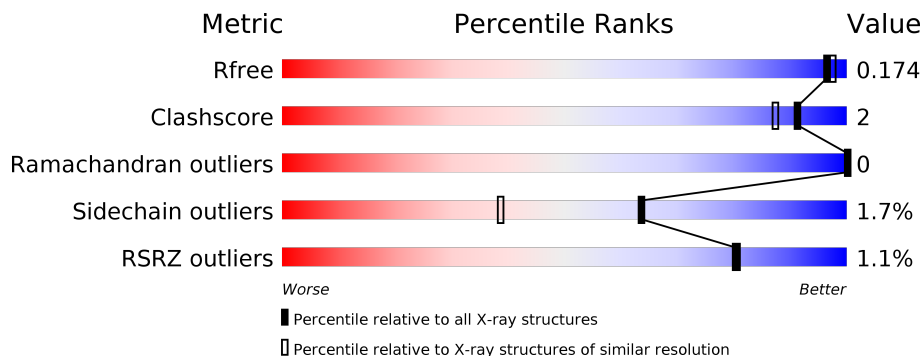
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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}	111664	3975 (1.64-1.60)
Clashscore	122126	4258 (1.64-1.60)
Ramachandran outliers	120053	4162 (1.64-1.60)
Sidechain outliers	120020	4161 (1.64-1.60)
RSRZ outliers	108989	3894 (1.64-1.60)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	474	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;">95% 5%</div> </div> </div>
1	B	474	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; text-align: center;">%</div> <div style="position: absolute; top: 10px; left: 0; width: 100%; text-align: center;">95% 5%</div> </div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16152 atoms, of which 7445 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
1	A	474	Total	C	H	N	O	S	0	9	0
			7388	2376	3640	652	702	18			
1	B	474	Total	C	H	N	O	S	0	10	0
			7399	2381	3643	653	705	17			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



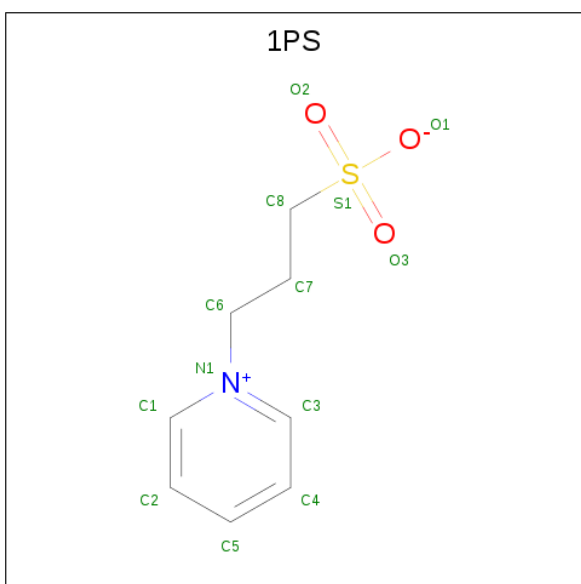
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	B	1	Total	C	H	O	0	0
			7	2	3	2		
3	B	1	Total	C	H	O	0	0
			7	2	3	2		
3	B	1	Total	C	H	O	0	0
			7	2	3	2		
3	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 4 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



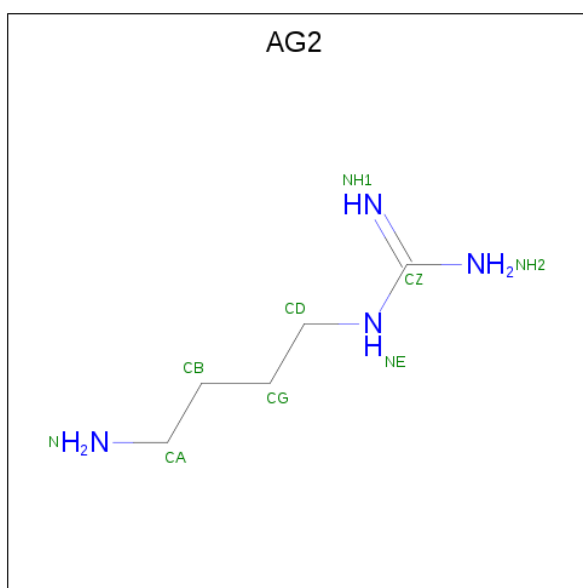
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 3-PYRIDINIUM-1-YLPROPANE-1-SULFONATE (three-letter code: 1PS) (formula: C₈H₁₁NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	S	
			24	8	11	1	3	1	
5	B	1	Total	C	H	N	O	S	
			24	8	11	1	3	1	
5	B	1	Total	C	H	N	O	S	
			24	8	11	1	3	1	
5	B	1	Total	C	H	N	O	S	
			24	8	11	1	3	1	

- Molecule 6 is AGMATINE (three-letter code: AG2) (formula: C₅H₁₄N₄).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	498	Total	O		
			498	498	0	0
7	B	486	Total	O		
			486	486	0	0

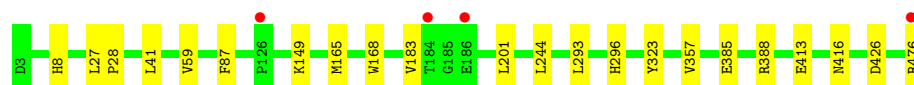
3 Residue-property plots [i](#)

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: Homospermidine synthase



- Molecule 1: Homospermidine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.86Å 108.56Å 161.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.63 90.06 – 1.63	Depositor EDS
% Data completeness (in resolution range)	98.2 (10.00-1.63) 93.9 (90.06-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.63Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.136 , 0.171 0.140 , 0.174	Depositor DCC
R_{free} test set	6019 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16152	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MHO, NAD, SO4, ACT, 1PS, AG2

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	0/3852	0.62	0/5249
1	B	0.44	0/3863	0.61	0/5263
All	All	0.44	0/7715	0.62	0/10512

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	3748	3640	3627	11	0
1	B	3756	3643	3630	12	0
2	A	44	26	26	0	0
2	B	44	26	26	0	0
3	A	12	9	9	0	0
3	B	20	15	15	2	0
4	A	15	0	0	0	0
4	B	5	0	0	0	0
5	A	13	11	11	0	0
5	B	39	33	33	0	0
6	A	9	14	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	18	28	26	2	0
7	A	498	0	0	6	9
7	B	486	0	0	10	6
All	All	8707	7445	7416	27	9

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 27 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:421:GLU:OE2	7:A:947:HOH:O	2.02	0.78
1:B:385[B]:GLU:OE1	1:B:388:ARG:NH2	2.17	0.77
1:A:220:LYS:O	7:A:1054:HOH:O	2.08	0.71
6:B:511:AG2:NE	7:B:1009:HOH:O	2.28	0.66
1:B:357[A]:VAL:O	7:B:1063:HOH:O	2.14	0.66

The worst 5 of 9 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:665:HOH:O	7:A:722:HOH:O[3_555]	2.05	0.15
7:A:687:HOH:O	7:B:856:HOH:O[4_555]	2.07	0.13
7:A:605:HOH:O	7:B:814:HOH:O[4_655]	2.11	0.09
7:A:707:HOH:O	7:B:848:HOH:O[1_455]	2.15	0.05
7:A:648:HOH:O	7:B:813:HOH:O[4_555]	2.15	0.05

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	480/474 (101%)	468 (98%)	12 (2%)	0	100	100
1	B	480/474 (101%)	466 (97%)	14 (3%)	0	100	100
All	All	960/948 (101%)	934 (97%)	26 (3%)	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	394/387 (102%)	387 (98%)	7 (2%)	62	36
1	B	396/387 (102%)	390 (98%)	6 (2%)	67	45
All	All	790/774 (102%)	777 (98%)	13 (2%)	63	42

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	HIS
1	A	323	TYR
1	B	293	LEU
1	A	293	LEU
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 ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	MHO	A	199	1	8,8,9	1.04	0	6,9,11	1.20	1 (16%)
1	MHO	B	199	1	8,8,9	0.96	0	6,9,11	1.55	1 (16%)

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
1	MHO	A	199	1	-	0/5/7/9	0/0/0/0
1	MHO	B	199	1	-	0/5/7/9	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	MHO	OD1-SD-CE	2.04	110.38	106.25
1	B	199	MHO	OD1-SD-CE	3.06	112.45	106.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

21 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	$\# Z > 2$
2	NAD	A	501	-	40,48,48	0.79	1 (2%)	44,73,73	1.56	6 (13%)
3	ACT	A	502	-	1,3,3	1.16	0	0,3,3	0.00	-
3	ACT	A	503	-	1,3,3	1.01	0	0,3,3	0.00	-
3	ACT	A	504	-	1,3,3	1.78	0	0,3,3	0.00	-
4	SO4	A	505	-	4,4,4	0.16	0	6,6,6	0.12	0
4	SO4	A	506	-	4,4,4	0.18	0	6,6,6	0.13	0
4	SO4	A	507	-	4,4,4	0.20	0	6,6,6	0.22	0
5	1PS	A	508	-	13,13,13	2.18	1 (7%)	15,17,17	1.19	1 (6%)
6	AG2	A	509	-	8,8,8	1.87	1 (12%)	7,8,8	0.49	0
2	NAD	B	501	-	40,48,48	0.81	3 (7%)	44,73,73	1.68	6 (13%)
3	ACT	B	502	-	1,3,3	1.20	0	0,3,3	0.00	-
3	ACT	B	503	-	1,3,3	1.01	0	0,3,3	0.00	-
3	ACT	B	504	-	1,3,3	2.11	1 (100%)	0,3,3	0.00	-
4	SO4	B	505	-	4,4,4	0.19	0	6,6,6	0.27	0
5	1PS	B	506	-	13,13,13	2.21	1 (7%)	15,17,17	1.23	1 (6%)
5	1PS	B	507	-	13,13,13	2.04	1 (7%)	15,17,17	1.42	2 (13%)
3	ACT	B	508	-	1,3,3	1.35	0	0,3,3	0.00	-
5	1PS	B	509	-	13,13,13	2.03	1 (7%)	15,17,17	1.45	2 (13%)
6	AG2	B	510	-	8,8,8	1.95	1 (12%)	7,8,8	0.82	0
6	AG2	B	511	-	8,8,8	1.79	1 (12%)	7,8,8	0.67	0
3	ACT	B	512	-	1,3,3	0.52	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	A	501	-	-	0/22/62/62	0/5/5/5
3	ACT	A	502	-	-	0/0/0/0	0/0/0/0
3	ACT	A	503	-	-	0/0/0/0	0/0/0/0
3	ACT	A	504	-	-	0/0/0/0	0/0/0/0
4	SO4	A	505	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	506	-	-	0/0/0/0	0/0/0/0
4	SO4	A	507	-	-	0/0/0/0	0/0/0/0
5	1PS	A	508	-	-	0/7/7/7	0/1/1/1
6	AG2	A	509	-	-	0/6/6/6	0/0/0/0
2	NAD	B	501	-	-	0/22/62/62	0/5/5/5
3	ACT	B	502	-	-	0/0/0/0	0/0/0/0
3	ACT	B	503	-	-	0/0/0/0	0/0/0/0
3	ACT	B	504	-	-	0/0/0/0	0/0/0/0
4	SO4	B	505	-	-	0/0/0/0	0/0/0/0
5	1PS	B	506	-	-	0/7/7/7	0/1/1/1
5	1PS	B	507	-	-	0/7/7/7	0/1/1/1
3	ACT	B	508	-	-	0/0/0/0	0/0/0/0
5	1PS	B	509	-	-	0/7/7/7	0/1/1/1
6	AG2	B	510	-	-	0/6/6/6	0/0/0/0
6	AG2	B	511	-	-	0/6/6/6	0/0/0/0
3	ACT	B	512	-	-	0/0/0/0	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	506	1PS	C8-S1	-7.72	1.66	1.77
5	A	508	1PS	C8-S1	-7.58	1.66	1.77
5	B	507	1PS	C8-S1	-7.06	1.67	1.77
5	B	509	1PS	C8-S1	-7.03	1.67	1.77
2	B	501	NAD	C8A-N9A	-2.39	1.34	1.36

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAD	N3A-C2A-N1A	-6.93	122.93	128.86
2	A	501	NAD	N3A-C2A-N1A	-6.24	123.53	128.86
2	B	501	NAD	C4B-O4B-C1B	-3.84	105.82	109.83
2	A	501	NAD	C4B-O4B-C1B	-3.01	106.69	109.83
2	B	501	NAD	C1B-N9A-C4A	-2.63	122.09	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	ACT	1	0
3	B	508	ACT	1	0
6	B	511	AG2	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	475:VAL	C	476[B]:ARG	N	2.91

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, 95th 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 ²)	Q<0.9
1	A	473/474 (99%)	-0.67	6 (1%) 77 76	10, 16, 36, 66	0
1	B	473/474 (99%)	-0.68	4 (0%) 86 86	11, 18, 37, 66	0
All	All	946/948 (99%)	-0.67	10 (1%) 80 80	10, 17, 36, 66	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	PHE	6.6
1	A	127	ASP	4.3
1	A	126	PRO	3.3
1	B	126	PRO	3.3
1	B	476[A]	ARG	2.9

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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 ²)	Q<0.9
1	MHO	B	199	9/10	0.98	0.06	16,20,33,48	0
1	MHO	A	199	9/10	0.99	0.07	11,16,40,58	0

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, 95th 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 ²)	Q<0.9
6	AG2	B	510	9/9	0.73	0.17	35,49,57,64	0
6	AG2	B	511	9/9	0.73	0.16	31,43,54,61	0
6	AG2	A	509	9/9	0.75	0.18	24,47,76,92	0
3	ACT	A	504	4/4	0.85	0.10	37,48,48,51	0
3	ACT	B	508	4/4	0.89	0.14	40,47,57,57	0
3	ACT	B	503	4/4	0.90	0.12	36,38,54,54	0
3	ACT	B	504	4/4	0.91	0.17	27,34,35,39	0
5	1PS	B	509	13/13	0.92	0.18	27,55,73,75	0
5	1PS	B	507	13/13	0.94	0.13	24,38,48,49	0
3	ACT	A	502	4/4	0.94	0.07	28,34,35,36	0
5	1PS	A	508	13/13	0.95	0.17	30,49,63,69	0
3	ACT	B	502	4/4	0.96	0.10	33,42,59,59	0
4	SO4	A	505	5/5	0.97	0.17	43,57,58,70	0
3	ACT	B	512	4/4	0.97	0.21	21,29,31,34	0
4	SO4	A	507	5/5	0.97	0.08	31,33,37,38	0
5	1PS	B	506	13/13	0.98	0.09	22,34,48,49	0
3	ACT	A	503	4/4	0.98	0.09	16,38,61,61	0
4	SO4	B	505	5/5	0.98	0.07	29,30,33,41	0
4	SO4	A	506	5/5	0.99	0.08	31,31,35,40	0
2	NAD	A	501	44/44	0.99	0.06	9,13,19,24	0
2	NAD	B	501	44/44	0.99	0.06	11,15,20,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.