



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 08:12 AM GMT

PDB ID : 1ABR  
Title : CRYSTAL STRUCTURE OF ABRIN-A  
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Deposited on : 1994-11-11  
Resolution : 2.14 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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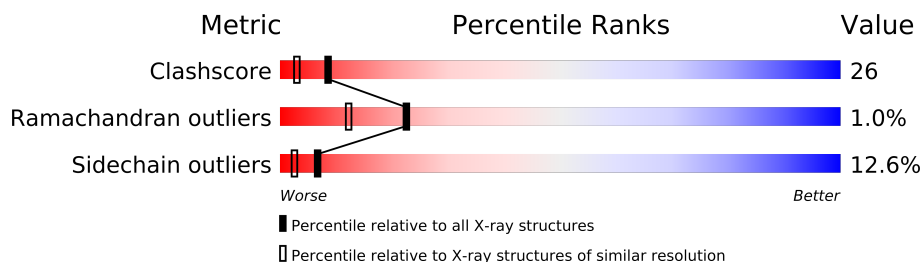
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	<b>FAILED</b>
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.14 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))
Clashscore	79885	1302 (2.16-2.12)
Ramachandran outliers	78287	1281 (2.16-2.12)
Sidechain outliers	78261	1281 (2.16-2.12)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	251	
2	B	267	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5798 atoms, of which 1387 are hydrogens and 0 are deuterium.

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 ABRIN-A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	251	Total	C	H	N	O	S	0	0	0
			2441	1242	458	349	388	4			

- Molecule 2 is a protein called ABRIN-A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	267	Total	C	H	N	O	S	0	0	0
			2603	1317	497	358	412	19			

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	5	Total	C	H	N	O	0	0
			77	34	16	2	25		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	5	Total	C	H	N	O	0	0
			77	34	16	2	25		

- Molecule 5 is water.

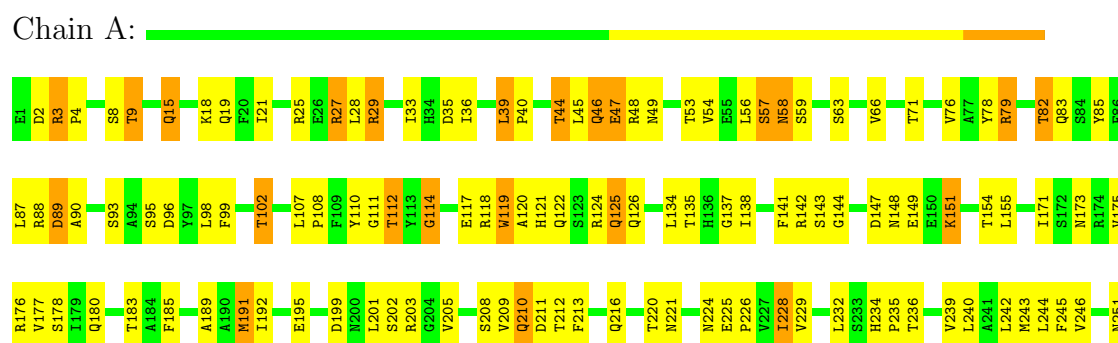
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	80	Total	H	O	0	0
			240	160	80		
5	B	120	Total	H	O	0	0
			360	240	120		

### 3 Residue-property plots

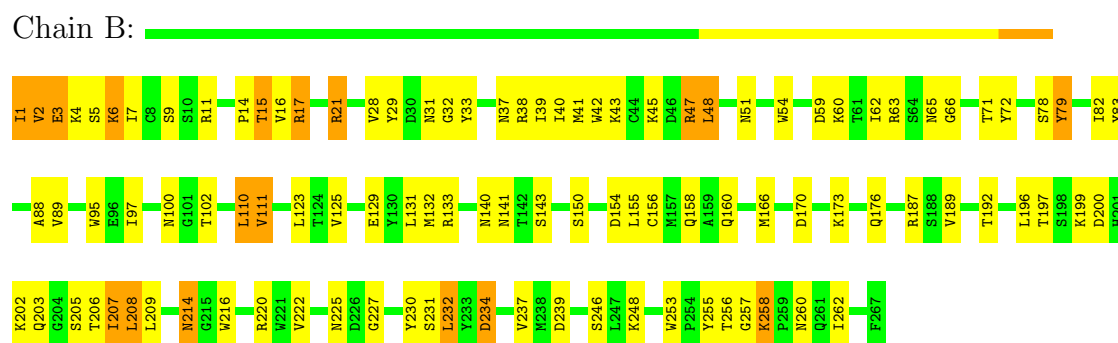
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS failed to run properly.

#### • Molecule 1: ABRIN-A



#### • Molecule 2: ABRIN-A



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.58Å 73.07Å 48.23Å 90.00° 96.20° 90.00°	Depositor
Resolution (Å)	10.00 – 2.14	Depositor
% Data completeness (in resolution range)	77.4 (10.00-2.14)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.15 (at 2.10Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.189 , (Not available)	Depositor
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.161	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 29019 reflections	Xtriage
Total number of atoms	5798	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, BMA, NGZ, NDG, MAN

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	0.59	0/2024	0.82	1/2755 (0.0%)
2	B	0.60	0/2153	0.85	2/2918 (0.1%)
All	All	0.60	0/4177	0.83	3/5673 (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
3	B	2	0
4	B	4	0
All	All	6	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	234	ASP	N-CA-C	-5.94	94.96	111.00
2	B	17	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	114	GLY	N-CA-C	-5.13	100.28	113.10

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	270(C)	MAN	C2,C1
4	B	274(D)	NDG	C5,C3,C1,C4

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1983	458	1474	125	0
2	B	2106	497	1528	92	0
3	B	61	16	36	6	0
4	B	61	16	36	18	0
5	A	80	160	0	9	0
5	B	120	240	0	7	0
All	All	4411	1387	3074	214	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 26.

The worst 5 of 214 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:48:LEU:HD23	4:B:274(D):NDG:H3	1.50	0.94
1:A:47:GLU:HG3	1:A:93:SER:HB2	1.49	0.91
1:A:147:ASP:HA	5:A:324:HOH:O	1.72	0.90
1:A:36:ILE:HB	5:A:329:HOH:O	1.77	0.84
1:A:243:MET:SD	5:A:329:HOH:O	2.35	0.84

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	249/251 (99%)	224 (90%)	21 (8%)	4 (2%)	14 5
2	B	265/267 (99%)	245 (92%)	19 (7%)	1 (0%)	43 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	514/518 (99%)	469 (91%)	40 (8%)	5 (1%)	22	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2	VAL
1	A	121	HIS
1	A	143	SER
1	A	47	GLU
1	A	3	ARG

### 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	219/219 (100%)	186 (85%)	33 (15%)	4	1
2	B	235/235 (100%)	211 (90%)	24 (10%)	11	5
All	All	454/454 (100%)	397 (87%)	57 (13%)	7	2

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	GLU
1	A	246	VAL
2	B	207	ILE
1	A	151	LYS
1	A	210	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
2	B	141	ASN
2	B	225	ASN
1	A	105	HIS

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Mol	Chain	Res	Type
2	B	176	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

10 carbohydrates 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	NDG	B	268(C)	3	12,14,15	0.77	0	15,19,21	1.11	2 (13%)
3	NGZ	B	269(C)	3	12,14,15	1.03	1 (8%)	15,19,21	0.79	1 (6%)
3	MAN	B	270(C)	3	10,11,12	1.26	1 (10%)	11,15,17	1.74	2 (18%)
3	MAN	B	271(C)	3	10,11,12	0.88	0	11,15,17	1.69	1 (9%)
3	BMA	B	272(C)	3	10,11,12	0.81	0	11,15,17	0.77	0
4	NDG	B	273(D)	4	12,14,15	0.92	1 (8%)	15,19,21	1.10	2 (13%)
4	NDG	B	274(D)	4	12,14,15	0.66	0	15,19,21	1.38	1 (6%)
4	BGC	B	275(D)	4	10,11,12	0.84	0	11,15,17	0.98	1 (9%)
4	MAN	B	276(D)	4	10,11,12	0.86	0	11,15,17	1.16	1 (9%)
4	BMA	B	277(D)	4	10,11,12	0.65	0	11,15,17	0.83	0

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	NDG	B	268(C)	3	-	0/6/23/26	1/1/1/1
3	NGZ	B	269(C)	3	-	0/6/23/26	1/1/1/1
3	MAN	B	270(C)	3	2/2/4/5	0/2/19/22	0/1/1/1
3	MAN	B	271(C)	3	-	0/2/19/22	0/1/1/1
3	BMA	B	272(C)	3	-	0/2/19/22	0/1/1/1
4	NDG	B	273(D)	4	-	0/6/23/26	0/1/1/1
4	NDG	B	274(D)	4	4/4/6/7	0/6/23/26	0/1/1/1
4	BGC	B	275(D)	4	-	0/2/19/22	0/1/1/1
4	MAN	B	276(D)	4	-	0/2/19/22	0/1/1/1
4	BMA	B	277(D)	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	270(C)	MAN	C3-C2	3.51	1.60	1.52
3	B	269(C)	NGZ	C4-C5	2.75	1.59	1.53
4	B	273(D)	NDG	C3-C2	2.48	1.57	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	271(C)	MAN	O5-C5-C6	5.37	112.62	106.98
4	B	274(D)	NDG	O-C5-C6	4.90	112.12	106.98
3	B	270(C)	MAN	O5-C5-C6	4.44	111.64	106.98
4	B	276(D)	MAN	O5-C5-C6	3.76	110.92	106.98
3	B	270(C)	MAN	C4-C3-C2	2.85	114.33	110.50

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	270(C)	MAN	C2
3	B	270(C)	MAN	C1
4	B	274(D)	NDG	C5
4	B	274(D)	NDG	C3
4	B	274(D)	NDG	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	268(C)	NDG	C1-C2-C3-C4-C5-O
3	B	269(C)	NGZ	C1-C2-C3-C4-C5-O5

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.