Full wwPDB X-ray Structure Validation Report ⓘ

Jul 26, 2023 – 03:04 AM EDT

PDB ID	:	1A4B
Title	:	AZURIN MUTANT WITH MET 121 REPLACED BY HIS, PH 6.5 CRYSTAL FORM, DATA COLLECTED AT-180 DEGREES CELSIUS
Authors	:	Messerschmidt, A.; Prade, L.
Deposited on	:	1998-01-28
Resolution	:	1.91 Å(reported)

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

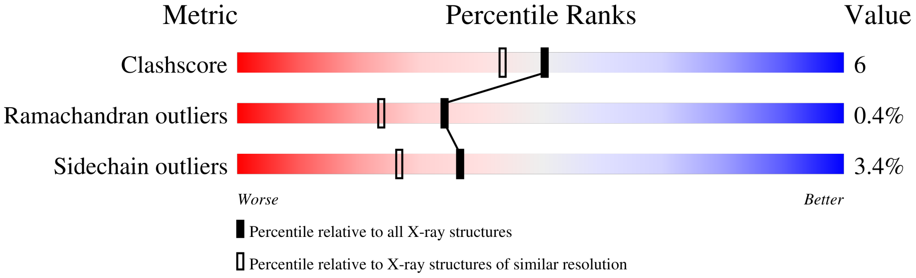
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.91 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	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	129	
1	B	129	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3475 atoms, of which 1152 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 AZURIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	129	1199	611	221	167	191	9	0	0	0
1	B	129	1199	611	221	167	191	9	0	0	0

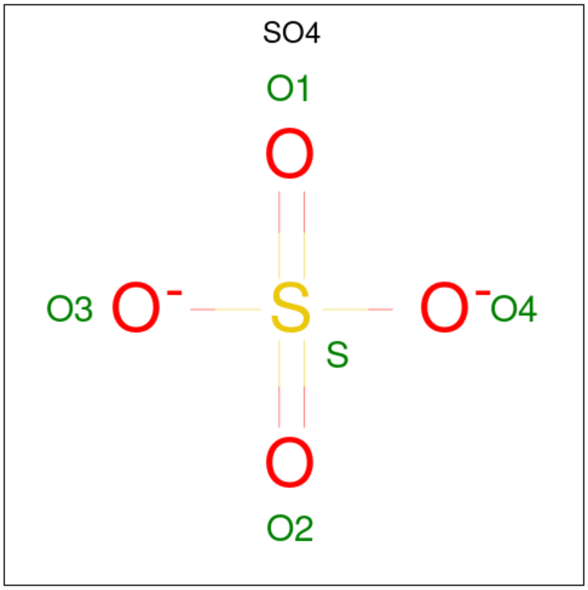
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ASP	ASN	conflict	UNP P00280
A	42	SER	VAL	SEE REMARK 999	UNP P00280
A	57	GLU	GLN	conflict	UNP P00280
A	121	HIS	MET	engineered mutation	UNP P00280
B	16	ASP	ASN	conflict	UNP P00280
B	42	SER	VAL	SEE REMARK 999	UNP P00280
B	57	GLU	GLN	conflict	UNP P00280
B	121	HIS	MET	engineered mutation	UNP P00280

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

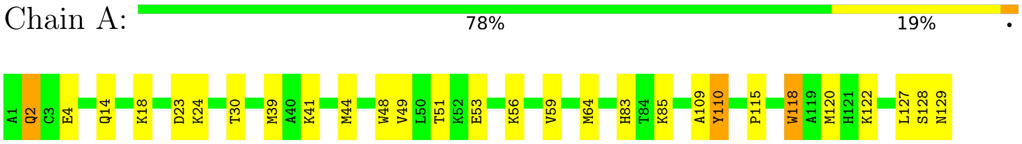
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	175	Total H O 525 350 175	0	0
4	B	180	Total H O 540 360 180	0	0

3 Residue-property plots ⓘ

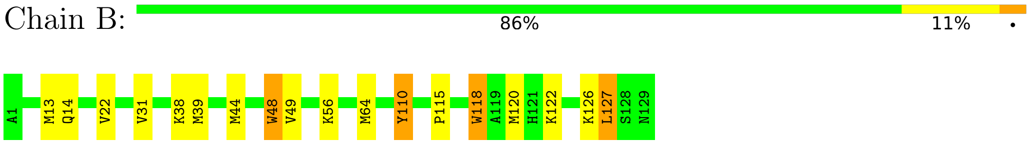
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: AZURIN



- Molecule 1: AZURIN



4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	**Value**	**Source**
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	74.56Å 73.57Å 97.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.91	Depositor
% Data completeness (in resolution range)	97.0 (8.00-1.91)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3475	wwPDB-VP
Average B, all atoms ($Å^2$)	18.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CU

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	0.74	0/997	1.34	12/1341 (0.9%)
1	B	0.76	0/997	1.35	9/1341 (0.7%)
All	All	0.75	0/1994	1.35	21/2682 (0.8%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	39	MET	CG-SD-CE	-10.29	83.74	100.20
1	B	48	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	A	48	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	A	39	MET	CA-CB-CG	-8.11	99.52	113.30
1	A	48	TRP	CE2-CD2-CG	-7.95	100.94	107.30
1	B	118	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	A	118	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	B	118	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	A	110	TYR	CB-CG-CD2	-7.35	116.59	121.00
1	B	48	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	A	48	TRP	CG-CD2-CE3	6.84	140.06	133.90
1	A	118	TRP	CE2-CD2-CG	-6.84	101.82	107.30
1	B	110	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	B	118	TRP	CG-CD2-CE3	5.88	139.19	133.90
1	A	127	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	48	TRP	CB-CG-CD1	-5.66	119.65	127.00
1	A	44	MET	CA-CB-CG	5.37	122.43	113.30
1	B	48	TRP	CG-CD1-NE1	-5.20	104.90	110.10
1	A	14	GLN	CA-CB-CG	5.14	124.70	113.40
1	B	118	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	A	118	TRP	CG-CD1-NE1	-5.01	105.09	110.10

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	978	221	950	11	2
1	B	978	221	950	12	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	175	350	0	1	0
4	B	180	360	0	1	1
All	All	2323	1152	1900	22	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 6.

All (22) 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:64:MET:HG3	1:B:115:PRO:HG3	1.74	0.70
1:B:56:LYS:NZ	1:B:122:LYS:HD3	2.14	0.62
1:A:4:GLU:HG2	1:A:30:THR:HB	1.84	0.59
1:B:56:LYS:HE2	1:B:118:TRP:HE3	1.68	0.58
1:B:120:MET:HB2	4:B:204:HOH:O	2.03	0.58
1:A:51:THR:HG21	1:A:59:VAL:HG21	1.85	0.57
1:B:13:MET:HB3	1:B:120:MET:HG2	1.91	0.53
1:A:83:HIS:HE1	4:A:163:HOH:O	1.94	0.51
1:A:49:VAL:O	1:A:110:TYR:HA	2.12	0.50
1:B:22:VAL:HB	1:B:127:LEU:HD12	1.96	0.48
1:A:24:LYS:HB2	1:A:129:ASN:HB3	1.96	0.47
1:A:23:ASP:HA	1:A:128:SER:O	2.14	0.47
1:B:49:VAL:O	1:B:110:TYR:HA	2.16	0.46
1:A:53:GLU:HG2	1:A:109:ALA:HB2	1.98	0.45
1:A:18:LYS:N	1:A:18:LYS:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:MET:HG3	1:B:44:MET:CE	2.49	0.43
1:A:56:LYS:HE2	1:A:118:TRP:HE3	1.85	0.42
1:B:56:LYS:HZ2	1:B:122:LYS:HD3	1.85	0.41
1:A:56:LYS:HE2	1:A:118:TRP:CE3	2.55	0.41
1:B:13:MET:CB	1:B:120:MET:HG2	2.50	0.40
1:B:31:VAL:HG21	1:B:48:TRP:CH2	2.56	0.40
1:B:56:LYS:HZ1	1:B:122:LYS:HD3	1.87	0.40

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)
1:A:122:LYS:HZ3	1:B:38:LYS:HZ1[4_555]	1.20	0.40
1:A:85:LYS:HZ2	4:B:274:HOH:H1[5_455]	1.32	0.28

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	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	9
1	B	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
All	All	254/258 (98%)	242 (95%)	11 (4%)	1 (0%)	34	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLN

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	103/103 (100%)	99 (96%)	4 (4%)	32	22
1	B	103/103 (100%)	100 (97%)	3 (3%)	42	33
All	All	206/206 (100%)	199 (97%)	7 (3%)	37	27

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	41	LYS
1	A	64	MET
1	A	115	PRO
1	B	14	GLN
1	B	126	LYS
1	B	127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	B	14	GLN
1	B	70	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 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	SO4	B	131	-	4,4,4	0.83	0	6,6,6	0.24	0
3	SO4	A	131	-	4,4,4	0.79	0	6,6,6	0.21	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.