



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6C9U / pdb_00006c9u
Title : Crystal structure of [KS3][AT3] didomain from module 3 of 6-deoxyerthronolide B synthase in complex with antibody fragment (Fab)
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Deposited on : 2018-01-28
Resolution : 2.09 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

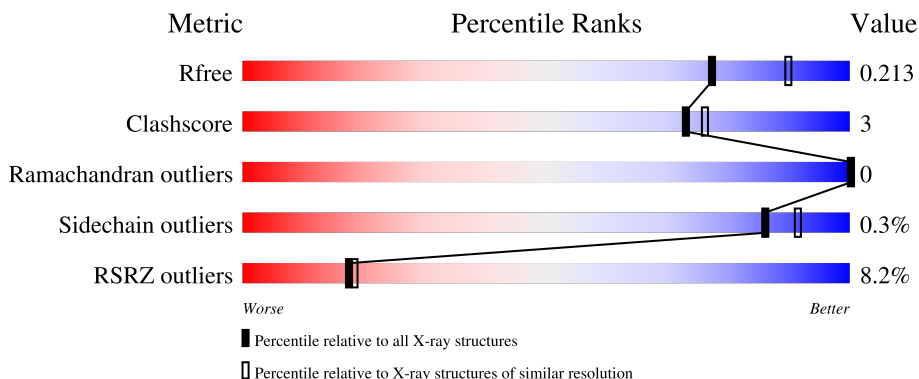
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	941	
2	L	236	
3	H	249	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20252 atoms, of which 9690 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 6-deoxyerythronolide-B synthase EryA2, modules 3 and 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	897	Total	C	H	N	O	S	0	7	0
			13357	4175	6615	1243	1305	19			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q03132
A	2	VAL	-	expression tag	UNP Q03132
A	439	ALA	ARG	conflict	UNP Q03132
A	481	SER	THR	conflict	UNP Q03132
A	924	SER	-	expression tag	UNP Q03132
A	925	SER	-	expression tag	UNP Q03132
A	926	SER	-	expression tag	UNP Q03132
A	927	VAL	-	expression tag	UNP Q03132
A	928	ASP	-	expression tag	UNP Q03132
A	929	LYS	-	expression tag	UNP Q03132
A	930	LEU	-	expression tag	UNP Q03132
A	931	ALA	-	expression tag	UNP Q03132
A	932	ALA	-	expression tag	UNP Q03132
A	933	ALA	-	expression tag	UNP Q03132
A	934	LEU	-	expression tag	UNP Q03132
A	935	GLU	-	expression tag	UNP Q03132
A	936	HIS	-	expression tag	UNP Q03132
A	937	HIS	-	expression tag	UNP Q03132
A	938	HIS	-	expression tag	UNP Q03132
A	939	HIS	-	expression tag	UNP Q03132
A	940	HIS	-	expression tag	UNP Q03132
A	941	HIS	-	expression tag	UNP Q03132

- Molecule 2 is a protein called Light chain of Fab 1B2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	209	Total	C	H	N	O	S	0	0	0
			3158	1001	1562	269	320	6			

- Molecule 3 is a protein called Heavy chain of Fab 1B2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	205	Total	C	H	N	O	S	0	0	0
			3052	978	1513	257	298	6			

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	460	Total	O	0	2
			462	462		
6	L	81	Total	O	0	0
			81	81		
6	H	139	Total	O	0	0
			139	139		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.77Å 139.68Å 102.58Å 90.00° 97.05° 90.00°	Depositor
Resolution (Å)	46.08 – 2.09 46.08 – 2.09	Depositor EDS
% Data completeness (in resolution range)	93.9 (46.08-2.09) 93.7 (46.08-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.166 , 0.210 0.170 , 0.213	Depositor DCC
R_{free} test set	2000 reflections (2.15%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20252	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, K, CSD

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	0/6867	0.65	0/9332
2	L	0.47	0/1630	0.59	0/2212
3	H	0.58	0/1575	0.65	0/2141
All	All	0.55	0/10072	0.64	0/13685

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 [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	6742	6615	6602	39	0
2	L	1596	1562	1561	18	0
3	H	1539	1513	1513	8	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
6	A	462	0	0	2	0
6	H	139	0	0	0	0
6	L	81	0	0	0	0
All	All	10562	9690	9676	63	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 3.

The worst 5 of 63 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:620:VAL:HG21	1:A:752:TYR:HE2	1.31	0.95
1:A:620:VAL:HG21	1:A:752:TYR:CE2	2.06	0.89
2:L:158:LEU:HD21	2:L:218:VAL:HG13	1.66	0.78
1:A:620:VAL:CG2	1:A:752:TYR:HE2	2.02	0.72
1:A:702:GLU:OE1	1:A:705:ARG:NH2	2.23	0.70

There are no symmetry-related clashes.

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	895/941 (95%)	854 (95%)	41 (5%)	0	100	100
2	L	203/236 (86%)	189 (93%)	14 (7%)	0	100	100
3	H	199/249 (80%)	195 (98%)	4 (2%)	0	100	100
All	All	1297/1426 (91%)	1238 (96%)	59 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	683/709 (96%)	682 (100%)	1 (0%)	88	93
2	L	185/208 (89%)	183 (99%)	2 (1%)	65	74
3	H	170/203 (84%)	170 (100%)	0	100	100
All	All	1038/1120 (93%)	1035 (100%)	3 (0%)	86	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
2	L	42	SER
2	L	130	ARG

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

Mol	Chain	Res	Type
2	L	182	GLN
3	H	41	GLN
3	H	171	HIS
1	A	491	GLN
1	A	559	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	CSD	A	203	1	4,7,8	0.84	0	1,8,10	1.50	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
1	CSD	A	203	1	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	203	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

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](#)

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	896/941 (95%)	0.06	59 (6%) 24 26	12, 40, 96, 143	6 (0%)
2	L	209/236 (88%)	0.67	27 (12%) 7 8	25, 59, 100, 114	0
3	H	205/249 (82%)	0.17	21 (10%) 12 12	22, 41, 97, 121	0
All	All	1310/1426 (91%)	0.17	107 (8%) 17 18	12, 43, 99, 143	6 (0%)

The worst 5 of 107 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	231	PHE	5.5
3	H	192	PRO	5.4
1	A	743	ILE	5.3
3	H	143	ALA	4.8
1	A	693	VAL	4.7

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	CSD	A	203	8/9	0.93	0.08	26,37,50,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	NA	A	1002	1/1	0.94	0.11	55,55,55,55	0
4	K	A	1001	1/1	0.99	0.06	37,37,37,37	0
5	NA	A	1003	1/1	1.00	0.04	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.