



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:01 AM UTC

PDB ID : 8EE1 / pdb_00008ee1
Title : KS-AT didomain from module 2 of the 6-deoxyerythronolide B synthase in complex with antibody fragment AA5
Authors : Cogan, D.P.; Brodsky, K.L.; Guzman, K.M.; Mathews, I.I.; Khosla, C.
Deposited on : 2022-09-06
Resolution : 2.70 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
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

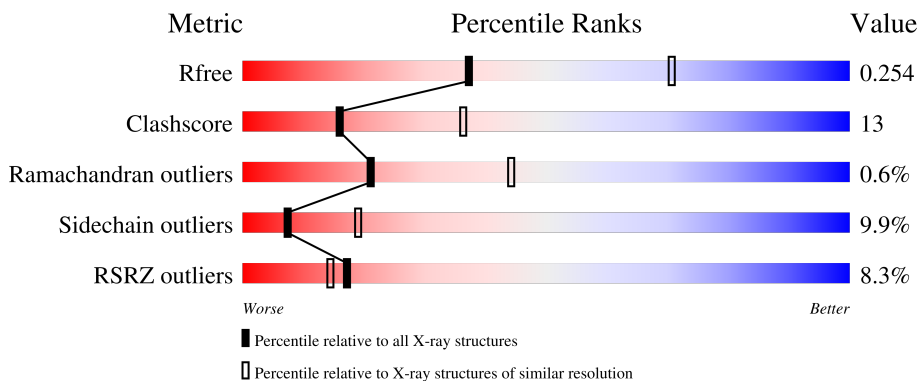
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	932	
1	D	932	
2	B	249	
2	G	249	
3	C	231	

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Mol	Chain	Length	Quality of chain
3	H	231	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (12%), a green segment (42%), a yellow segment (18%), and a grey segment (38%). The percentages are labeled below the bar. A small black dot is visible on the grey segment.</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17757 atoms, of which 0 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	840	6094	3800	1100	1173	21	0	0	0
1	D	846	6105	3802	1094	1188	21	0	0	0

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q5UNP6
A	2	ALA	-	expression tag	UNP Q5UNP6
A	3	SER	-	expression tag	UNP Q5UNP6
A	4	THR	-	expression tag	UNP Q5UNP6
A	5	ASP	-	expression tag	UNP Q5UNP6
A	6	SER	-	expression tag	UNP Q5UNP6
A	7	GLU	-	expression tag	UNP Q5UNP6
A	8	LYS	-	expression tag	UNP Q5UNP6
A	9	VAL	-	expression tag	UNP Q5UNP6
A	10	ALA	-	expression tag	UNP Q5UNP6
A	11	GLU	-	expression tag	UNP Q5UNP6
A	12	TYR	-	expression tag	UNP Q5UNP6
A	13	LEU	-	expression tag	UNP Q5UNP6
A	14	ARG	-	expression tag	UNP Q5UNP6
A	15	ARG	-	expression tag	UNP Q5UNP6
A	16	ALA	-	expression tag	UNP Q5UNP6
A	17	THR	-	expression tag	UNP Q5UNP6
A	18	LEU	-	expression tag	UNP Q5UNP6
A	19	ASP	-	expression tag	UNP Q5UNP6
A	20	LEU	-	expression tag	UNP Q5UNP6
A	21	ARG	-	expression tag	UNP Q5UNP6
A	22	ALA	-	expression tag	UNP Q5UNP6
A	23	ALA	-	expression tag	UNP Q5UNP6
A	24	ARG	-	expression tag	UNP Q5UNP6
A	25	GLN	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ARG	-	expression tag	UNP Q5UNP6
A	27	ILE	-	expression tag	UNP Q5UNP6
A	28	ARG	-	expression tag	UNP Q5UNP6
A	29	GLU	-	expression tag	UNP Q5UNP6
A	30	LEU	-	expression tag	UNP Q5UNP6
A	31	GLU	-	expression tag	UNP Q5UNP6
A	32	SER	-	expression tag	UNP Q5UNP6
A	922	ALA	-	expression tag	UNP Q5UNP6
A	923	ALA	-	expression tag	UNP Q5UNP6
A	924	ALA	-	expression tag	UNP Q5UNP6
A	925	LEU	-	expression tag	UNP Q5UNP6
A	926	GLU	-	expression tag	UNP Q5UNP6
A	927	HIS	-	expression tag	UNP Q5UNP6
A	928	HIS	-	expression tag	UNP Q5UNP6
A	929	HIS	-	expression tag	UNP Q5UNP6
A	930	HIS	-	expression tag	UNP Q5UNP6
A	931	HIS	-	expression tag	UNP Q5UNP6
A	932	HIS	-	expression tag	UNP Q5UNP6
D	1	MET	-	expression tag	UNP Q5UNP6
D	2	ALA	-	expression tag	UNP Q5UNP6
D	3	SER	-	expression tag	UNP Q5UNP6
D	4	THR	-	expression tag	UNP Q5UNP6
D	5	ASP	-	expression tag	UNP Q5UNP6
D	6	SER	-	expression tag	UNP Q5UNP6
D	7	GLU	-	expression tag	UNP Q5UNP6
D	8	LYS	-	expression tag	UNP Q5UNP6
D	9	VAL	-	expression tag	UNP Q5UNP6
D	10	ALA	-	expression tag	UNP Q5UNP6
D	11	GLU	-	expression tag	UNP Q5UNP6
D	12	TYR	-	expression tag	UNP Q5UNP6
D	13	LEU	-	expression tag	UNP Q5UNP6
D	14	ARG	-	expression tag	UNP Q5UNP6
D	15	ARG	-	expression tag	UNP Q5UNP6
D	16	ALA	-	expression tag	UNP Q5UNP6
D	17	THR	-	expression tag	UNP Q5UNP6
D	18	LEU	-	expression tag	UNP Q5UNP6
D	19	ASP	-	expression tag	UNP Q5UNP6
D	20	LEU	-	expression tag	UNP Q5UNP6
D	21	ARG	-	expression tag	UNP Q5UNP6
D	22	ALA	-	expression tag	UNP Q5UNP6
D	23	ALA	-	expression tag	UNP Q5UNP6
D	24	ARG	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	25	GLN	-	expression tag	UNP Q5UNP6
D	26	ARG	-	expression tag	UNP Q5UNP6
D	27	ILE	-	expression tag	UNP Q5UNP6
D	28	ARG	-	expression tag	UNP Q5UNP6
D	29	GLU	-	expression tag	UNP Q5UNP6
D	30	LEU	-	expression tag	UNP Q5UNP6
D	31	GLU	-	expression tag	UNP Q5UNP6
D	32	SER	-	expression tag	UNP Q5UNP6
D	922	ALA	-	expression tag	UNP Q5UNP6
D	923	ALA	-	expression tag	UNP Q5UNP6
D	924	ALA	-	expression tag	UNP Q5UNP6
D	925	LEU	-	expression tag	UNP Q5UNP6
D	926	GLU	-	expression tag	UNP Q5UNP6
D	927	HIS	-	expression tag	UNP Q5UNP6
D	928	HIS	-	expression tag	UNP Q5UNP6
D	929	HIS	-	expression tag	UNP Q5UNP6
D	930	HIS	-	expression tag	UNP Q5UNP6
D	931	HIS	-	expression tag	UNP Q5UNP6
D	932	HIS	-	expression tag	UNP Q5UNP6

- Molecule 2 is a protein called AA5 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	1583	1005	261	312	5	0	0	0
2	G	165	1260	800	213	244	3	0	0	0

- Molecule 3 is a protein called AA5 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	205	1562	973	265	319	5	0	0	0
3	H	144	1079	672	180	223	4	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O 1 1	0	0
4	C	4	Total O 4 4	0	0
4	D	29	Total O 29 29	0	0

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	249.37Å 252.44Å 63.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.62 – 2.70 39.62 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.62-2.70) 92.0 (39.62-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.225 , 0.254 0.225 , 0.254	Depositor DCC
R_{free} test set	5514 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	68.1	Xtrriage
Anisotropy	0.235	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.008 for k,h,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17757	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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](#)

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	0.60	0/6215	0.84	1/8470 (0.0%)
1	D	0.59	0/6222	0.79	1/8483 (0.0%)
2	B	0.54	0/1624	0.78	0/2217
2	G	0.58	0/1292	0.81	1/1756 (0.1%)
3	C	0.57	0/1596	0.79	1/2169 (0.0%)
3	H	0.62	0/1101	0.86	0/1496
All	All	0.59	0/18050	0.81	4/24591 (0.0%)

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
1	A	0	5
1	D	0	2
2	B	0	1
2	G	0	1
All	All	0	9

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	102	GLY	CA-C-O	-6.12	118.24	122.22
1	D	741	GLU	N-CA-C	-5.60	106.15	112.87
1	A	768	LEU	N-CA-C	-5.33	105.55	111.36
3	C	83	GLY	CA-C-O	-5.28	118.52	122.37

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	ARG	Sidechain
1	A	677	ARG	Sidechain
1	A	682	ARG	Sidechain
1	A	72	ARG	Sidechain
1	A	748	ARG	Sidechain

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	6094	0	5935	123	0
1	D	6105	0	5918	150	0
2	B	1583	0	1540	59	0
2	G	1260	0	1218	55	0
3	C	1562	0	1487	50	0
3	H	1079	0	1007	35	0
4	A	40	0	0	1	0
4	B	1	0	0	0	0
4	C	4	0	0	1	0
4	D	29	0	0	1	0
All	All	17757	0	17105	460	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 13.

The worst 5 of 460 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:D:690:MET:HG3	1:D:752:VAL:HG21	1.57	0.85
1:D:619:ARG:HH22	1:D:682:ARG:HH11	1.25	0.85
1:D:604:VAL:HG13	1:D:606:GLU:HG2	1.57	0.84
1:D:353:LEU:HD22	1:D:419:ILE:HD12	1.62	0.81
1:A:596:LEU:HB2	1:A:671:MET:HE3	1.65	0.79

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	832/932 (89%)	773 (93%)	54 (6%)	5 (1%)	21	44
1	D	836/932 (90%)	772 (92%)	59 (7%)	5 (1%)	21	44
2	B	206/249 (83%)	189 (92%)	17 (8%)	0	100	100
2	G	157/249 (63%)	140 (89%)	15 (10%)	2 (1%)	9	25
3	C	201/231 (87%)	183 (91%)	18 (9%)	0	100	100
3	H	138/231 (60%)	124 (90%)	12 (9%)	2 (1%)	9	23
All	All	2370/2824 (84%)	2181 (92%)	175 (7%)	14 (1%)	21	44

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	156	PRO
3	H	154	ASN
1	A	600	ALA
1	A	603	SER
3	H	85	GLY

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	605/690 (88%)	556 (92%)	49 (8%)	11	27
1	D	606/690 (88%)	547 (90%)	59 (10%)	8	20
2	B	180/206 (87%)	159 (88%)	21 (12%)	5	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	141/206 (68%)	118 (84%)	23 (16%)	2 6
3	C	173/199 (87%)	155 (90%)	18 (10%)	7 17
3	H	116/199 (58%)	106 (91%)	10 (9%)	10 25
All	All	1821/2190 (83%)	1641 (90%)	180 (10%)	7 19

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	468	ARG
1	D	861	ASP
1	D	481	SER
1	D	701	GLU
2	G	32	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	172	GLN
1	D	624	GLN
1	D	498	HIS
1	D	806	ASN
2	B	8	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [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	840/932 (90%)	0.23	39 (4%) 37 34	44, 66, 101, 133	0
1	D	846/932 (90%)	0.32	60 (7%) 22 19	43, 69, 120, 162	0
2	B	212/249 (85%)	0.97	26 (12%) 8 7	64, 95, 119, 154	0
2	G	165/249 (66%)	0.91	22 (13%) 7 6	68, 90, 139, 185	0
3	C	205/231 (88%)	0.86	27 (13%) 7 6	61, 93, 145, 150	0
3	H	144/231 (62%)	1.09	27 (18%) 3 3	70, 98, 141, 170	0
All	All	2412/2824 (85%)	0.48	201 (8%) 17 14	43, 75, 126, 185	0

The worst 5 of 201 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	185	LEU	6.2
3	H	194	SER	6.1
1	A	697	ARG	5.5
1	D	74	TRP	5.4
3	H	180	VAL	5.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.