

wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 01:42 AM EDT

PDB ID	:	8EE1
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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

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.



Motria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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 cha	in		
1	А	932	3% 69%			19%	• 10%
1	D	932	5% 66%			22%	• 9%
2	В	249	7% 50%		32%	·	15%
2	G	249	37%	25%	•	34%	
3	С	231	10%		27%	6	• 11%



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Mol	Chain	Length			Quality	y of ch	ain	
			12%					
3	Н	231		43%		17%	•	38%



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.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
1	А	840	Total	C 2800	N 1100	0_{1172}	S 21	0	0	0
			0094	3000	1100	1179	Z1			
1	Л	846	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	D	040	6105	3802	1094	1188	88 21	0	0	0

• Molecule 1 is a protein called 6-deoxyerythronolide B synthase.

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

There are 86 discrepancies between the modelled and reference sequences:



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Residue	Modelled	Actual	Comment	Reference
26	ARG	-	expression tag	UNP Q5UNP6
27	ILE	-	expression tag	UNP Q5UNP6
28	ARG	-	expression tag	UNP Q5UNP6
29	GLU	-	expression tag	UNP Q5UNP6
30	LEU	-	expression tag	UNP Q5UNP6
31	GLU	-	expression tag	UNP Q5UNP6
32	SER	-	expression tag	UNP Q5UNP6
922	ALA	-	expression tag	UNP Q5UNP6
923	ALA	-	expression tag	UNP Q5UNP6
924	ALA	-	expression tag	UNP Q5UNP6
925	LEU	-	expression tag	UNP Q5UNP6
926	GLU	-	expression tag	UNP Q5UNP6
927	HIS	-	expression tag	UNP Q5UNP6
928	HIS	-	expression tag	UNP Q5UNP6
929	HIS	-	expression tag	UNP Q5UNP6
930	HIS	_	expression tag	UNP Q5UNP6
931	HIS	_	expression tag	UNP Q5UNP6
932	HIS	_	expression tag	UNP Q5UNP6
1	MET	_	expression tag	UNP Q5UNP6
2	ALA	_	expression tag	UNP Q5UNP6
3	SER	_	expression tag	UNP Q5UNP6
4	THR	_	expression tag	UNP Q5UNP6
5	ASP	_	expression tag	UNP Q5UNP6
6	SER	_	expression tag	UNP Q5UNP6
7	GLU	_	expression tag	UNP Q5UNP6
8	LYS	-	expression tag	UNP Q5UNP6
9	VAL	_	expression tag	UNP Q5UNP6
10	ALA	-	expression tag	UNP Q5UNP6
11	GLU	_	expression tag	UNP Q5UNP6
12	TYR	-	expression tag	UNP Q5UNP6
13	LEU	-	expression tag	UNP Q5UNP6
14	ARG	-	expression tag	UNP Q5UNP6
15	ARG	-	expression tag	UNP Q5UNP6
16	ALA	-	expression tag	UNP Q5UNP6
17	THR	-	expression tag	UNP Q5UNP6
18	LEU	-	expression tag	UNP Q5UNP6
19	ASP	-	expression tag	UNP Q5UNP6
20	LEU	-	expression tag	UNP Q5UNP6
21	ARG	-	expression tag	UNP Q5UNP6
22	ALA	-	expression tag	UNP Q5UNP6
23	ALA	-	expression tag	UNP Q5UNP6
24	ARG	_	expression tag	UNP Q5UNP6
	Residue 26 27 28 29 30 31 32 922 923 924 925 926 927 928 929 930 931 932 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23	Residue Modelled 26 ARG 27 ILE 28 ARG 29 GLU 30 LEU 31 GLU 32 SER 922 ALA 923 ALA 924 ALA 925 LEU 926 GLU 927 HIS 928 HIS 929 HIS 930 HIS 931 HIS 932 HIS 933 SER 4 THR 5 ASP 6 SER 7 GLU 8 LYS 9 VAL 10 ALA 11 GLU 12 TYR 13 LEU 14 ARG 15 ARG 16 ALA 17 THR <td>Residue Modelled Actual 26 ARG - 27 ILE - 28 ARG - 29 GLU - 30 LEU - 31 GLU - 32 SER - 922 ALA - 923 ALA - 924 ALA - 925 LEU - 926 GLU - 927 HIS - 928 HIS - 929 HIS - 930 HIS - 931 HIS - 932 HIS - 1 MET - 2 ALA - 3 SER - 1 MET - 1 MET - 1 GLU - 8 LYS</td> <td>ResidueModelledActualComment26ARG-expression tag27ILE-expression tag28ARG-expression tag29GLU-expression tag30LEU-expression tag31GLU-expression tag32SER-expression tag922ALA-expression tag923ALA-expression tag924ALA-expression tag925LEU-expression tag926GLU-expression tag927HIS-expression tag928HIS-expression tag929HIS-expression tag930HIS-expression tag931HIS-expression tag1MET-expression tag2ALA-expression tag1MET-expression tag1</td>	Residue Modelled Actual 26 ARG - 27 ILE - 28 ARG - 29 GLU - 30 LEU - 31 GLU - 32 SER - 922 ALA - 923 ALA - 924 ALA - 925 LEU - 926 GLU - 927 HIS - 928 HIS - 929 HIS - 930 HIS - 931 HIS - 932 HIS - 1 MET - 2 ALA - 3 SER - 1 MET - 1 MET - 1 GLU - 8 LYS	ResidueModelledActualComment26ARG-expression tag27ILE-expression tag28ARG-expression tag29GLU-expression tag30LEU-expression tag31GLU-expression tag32SER-expression tag922ALA-expression tag923ALA-expression tag924ALA-expression tag925LEU-expression tag926GLU-expression tag927HIS-expression tag928HIS-expression tag929HIS-expression tag930HIS-expression tag931HIS-expression tag1MET-expression tag2ALA-expression tag1MET-expression tag1

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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

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	212	Total	С	Ν	0	\mathbf{S}	0	0	0
_	D		1583	1005	261	312	5		0	Ŭ
9	C	165	Total	С	Ν	0	\mathbf{S}	0	0	0
	G	105	1260	800	213	244	3	0	0	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
3	С	205	Total C	Total C N O S	0	0	0			
5	3 0	205	1562	973	265	319	5	0		0
2	ц	144	Total	С	Ν	0	S	0	0	0
5	о п	144	1079	672	180	223	4	0	0	

• Molecule 4 is water.

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



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total O 1 1	0	0
4	С	4	Total O 4 4	0	0
4	D	29	TotalO2929	0	0



3 Residue-property plots (i)

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 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: 6-deoxyerythronolide B synthase





• Molecule 2: AA5 antibody heavy chain



• Molecule 2: AA5 antibody heavy chain







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	249.37Å 252.44 Å 63.92 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	39.62 - 2.70	Depositor
Resolution (A)	39.62 - 2.70	EDS
% Data completeness	98.3 (39.62-2.70)	Depositor
(in resolution range)	92.0 (39.62-2.70)	EDS
R _{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.43 (at 2.69 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.225 , 0.254	Depositor
Λ, Λ_{free}	0.226 , 0.253	DCC
R_{free} test set	5514 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	68.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , 54.3	EDS
L-test for $twinning^2$	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
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

Xtriage'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.

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.



¹Intensities estimated from amplitudes.

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	
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.54	0/6215	0.72	0/8470
1	D	0.55	0/6222	0.72	0/8483
2	В	0.51	0/1624	0.67	0/2217
2	G	0.50	0/1292	0.67	0/1756
3	С	0.48	0/1596	0.65	0/2169
3	Н	0.51	0/1101	0.71	0/1496
All	All	0.53	0/18050	0.71	0/24591

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	А	0	5
1	D	0	2
2	В	0	1
2	G	0	1
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	243	ARG	Sidechain
1	А	677	ARG	Sidechain
1	А	682	ARG	Sidechain
1	А	72	ARG	Sidechain
1	А	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	А	6094	0	5935	114	0
1	D	6105	0	5918	135	0
2	В	1583	0	1540	57	0
2	G	1260	0	1218	49	0
3	С	1562	0	1487	47	0
3	Н	1079	0	1007	34	0
4	А	40	0	0	1	0
4	В	1	0	0	0	0
4	С	4	0	0	1	0
4	D	29	0	0	0	0
All	All	17757	0	17105	424	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 12.

The worst 5 of 424 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:298:GLN:HG3	1:A:300:GLY:H	1.48	0.76

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	832/932~(89%)	773~(93%)	54 (6%)	5 (1%)	25	50
1	D	836/932~(90%)	772 (92%)	59 (7%)	5 (1%)	25	50
2	В	206/249~(83%)	189 (92%)	17 (8%)	0	100	100
2	G	157/249~(63%)	140 (89%)	15 (10%)	2(1%)	12	30
3	С	201/231~(87%)	183 (91%)	18 (9%)	0	100	100
3	Н	138/231~(60%)	124 (90%)	12 (9%)	2(1%)	11	28
All	All	2370/2824~(84%)	2181 (92%)	175 (7%)	14 (1%)	25	50

analysed, and the total number of residues.

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	156	PRO
3	Н	154	ASN
1	А	600	ALA
1	А	603	SER
3	Н	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	Perce	ntiles
1	А	605/690~(88%)	565~(93%)	40 (7%)	16	38
1	D	606/690~(88%)	546 (90%)	60 (10%)	8	18
2	В	180/206~(87%)	159 (88%)	21 (12%)	5	12
2	G	141/206~(68%)	117 (83%)	24 (17%)	2	5
3	С	173/199~(87%)	156 (90%)	17 (10%)	8	18
3	Н	116/199~(58%)	104 (90%)	12 (10%)	7	16
All	All	1821/2190 (83%)	1647 (90%)	174 (10%)	8	19

5 of 174 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	D	639	ARG
2	G	64	SER
1	D	710	THR
1	D	815	SER
2	G	103	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	С	206	HIS
1	D	498	HIS
3	Н	155	ASN
1	D	731	GLN
1	D	806	ASN

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 monosaccharides 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, 95^{th} 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	А	840/932~(90%)	0.08	26 (3%) 49 49	44, 66, 101, 133	0
1	D	846/932~(90%)	0.20	44 (5%) 27 25	43, 69, 120, 162	0
2	В	212/249~(85%)	0.47	17 (8%) 12 10	64, 95, 119, 154	0
2	G	165/249~(66%)	0.49	20 (12%) 4 3	68, 90, 139, 185	0
3	С	205/231~(88%)	0.52	23 (11%) 5 4	61, 93, 145, 150	0
3	Н	144/231~(62%)	0.79	27 (18%) 1 0	70, 98, 141, 170	0
All	All	2412/2824 (85%)	0.26	157 (6%) 18 17	43, 75, 126, 185	0

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	С	222	VAL	5.4
1	D	713	LEU	5.2
3	Н	181	THR	4.9
3	Н	179	SER	4.7
2	G	216	LYS	4.7

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 monosaccharides 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.

