



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:11 AM UTC

PDB ID : 6ULW / pdb_00006ulw
Title : Adenylation, ketoreductase, and pseudo A-sub multidomain structure of a keto acid-selecting NRPS module
Authors : Alonzo, D.A.; Wang, J.; Chiche-Lapierre, C.; Schmeing, T.M.
Deposited on : 2019-10-08
Resolution : 3.40 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

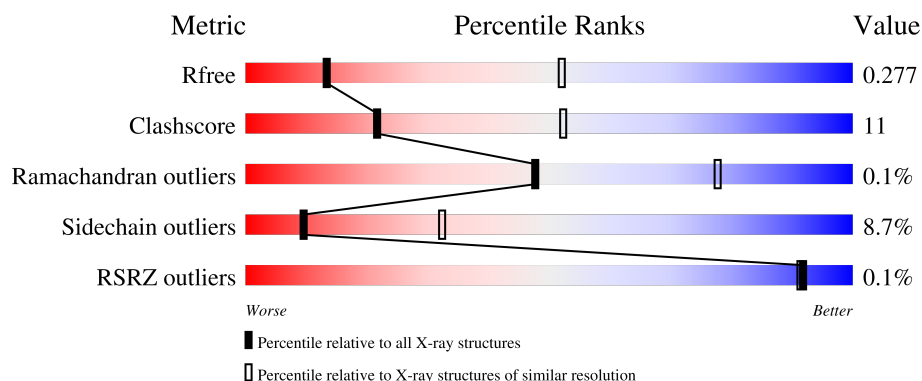
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	1327	 67% 21% • 10%
1	B	1327	 66% 22% • 9%
1	C	1327	 66% 22% • 9%
1	D	1327	 67% 21% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 74888 atoms, of which 37048 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 Amino acid adenylation domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1193	Total	C	H	N	O	S	0	0	0
			18613	5974	9210	1598	1782	49			
1	B	1209	Total	C	H	N	O	S	0	0	0
			18852	6049	9327	1618	1808	50			
1	C	1203	Total	C	H	N	O	S	0	0	0
			18783	6024	9294	1613	1803	49			
1	D	1193	Total	C	H	N	O	S	0	0	0
			18631	5979	9217	1600	1786	49			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1319	ALA	-	expression tag	UNP M5R382
A	1320	ALA	-	expression tag	UNP M5R382
A	1321	ALA	-	expression tag	UNP M5R382
A	1322	GLU	-	expression tag	UNP M5R382
A	1323	ASN	-	expression tag	UNP M5R382
A	1324	LEU	-	expression tag	UNP M5R382
A	1325	TYR	-	expression tag	UNP M5R382
A	1326	PHE	-	expression tag	UNP M5R382
A	1327	GLN	-	expression tag	UNP M5R382
B	1319	ALA	-	expression tag	UNP M5R382
B	1320	ALA	-	expression tag	UNP M5R382
B	1321	ALA	-	expression tag	UNP M5R382
B	1322	GLU	-	expression tag	UNP M5R382
B	1323	ASN	-	expression tag	UNP M5R382
B	1324	LEU	-	expression tag	UNP M5R382
B	1325	TYR	-	expression tag	UNP M5R382
B	1326	PHE	-	expression tag	UNP M5R382
B	1327	GLN	-	expression tag	UNP M5R382
C	1319	ALA	-	expression tag	UNP M5R382
C	1320	ALA	-	expression tag	UNP M5R382
C	1321	ALA	-	expression tag	UNP M5R382

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1322	GLU	-	expression tag	UNP M5R382
C	1323	ASN	-	expression tag	UNP M5R382
C	1324	LEU	-	expression tag	UNP M5R382
C	1325	TYR	-	expression tag	UNP M5R382
C	1326	PHE	-	expression tag	UNP M5R382
C	1327	GLN	-	expression tag	UNP M5R382
D	1319	ALA	-	expression tag	UNP M5R382
D	1320	ALA	-	expression tag	UNP M5R382
D	1321	ALA	-	expression tag	UNP M5R382
D	1322	GLU	-	expression tag	UNP M5R382
D	1323	ASN	-	expression tag	UNP M5R382
D	1324	LEU	-	expression tag	UNP M5R382
D	1325	TYR	-	expression tag	UNP M5R382
D	1326	PHE	-	expression tag	UNP M5R382
D	1327	GLN	-	expression tag	UNP M5R382

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0
2	D	2	Total Ca 2 2	0	0

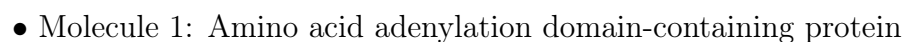
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0

- Molecule 1: Amino acid adenylation domain-containing protein



MET	LVS	PRO	SER	THR	ILF	ASW	GLN	THR	SER	ARG	HTS	E13	S14	M15	V22	K23	T24	L27	Q28	T29	E33	R34	F35	F38	K42	I44	H50	L51	L54	F55	L56	E63	E67	T71	GLN	LVS	ALA	VAL	PRO	PRO	ALA	LEU	ALA	ASP	MET	PRO	P83	A84	L85
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V408	\$255	ALA	MET
M415	V256	ASP	LYS
S416	L260	MET	PRO
E417		PRO	SER
I418	S264	P83	THR
S419		A84	ILE
S420	V271	L85	ASN
A421	V272	S86	GLN
A422	E273	Y87	THR
V423			SER
A427	L279	L91	ARG
I428		D92	His
D432	V282	T99	E13
	T285	L100	D21
S435		Q101	V22
L438	T292	T125	T25
T439	V296	D134	Q28
E442	S297	R137	T29
L445	T306		N30
T446	T309	Q156	V37
A452	F312	L179	F38
R455	T324	V180	S39
E464	T332	N190	R40
L465	L336		E41
G466	R346	M190	K42
K467		V193	T43
P468	N354	K195	I44
I469	D362	W200	
I472	T367	H205	Y49
T476	L374	T208	H50
M478	S375	L209	L51
H479	A376	T210	S82
Q480			H83
L483	N382	E215	L54
L484	G383	E216	F55
P485	K384	E217	
E486	E385	V218	K38
D487	K386	T227	
H488	V387	Q229	ALA
	V388	L230	ILE
K495		R231	GLN
		V232	THR
M500	L398	T240	GLN
Y503	H402	A250	LYS
A509	K405	A251	ALA
			VAL
			PRO
			ALA
			THR
			LEU

GLN	GLY	HIS	SER	LEU	LYS	ALA	THR	GLN	MET	LEU	SER	ALA	VAL	ARG	GLN	LYS	THR	GLY	PHE	ASP	VAL	PRO	LEU	ALA	VAL	LEU	PHE	GLU	HIS	THR	ARG	LEU	GLY	GLU	LEU	ALA	ASP	TRP	ILE	ASP	SER	ASN	ALA	LYS	ALA	ASP	GLU	VAL	ILE	ASP	PRO	MET	VAL	GLY	TYR	PHE						
	E1178	R1179		R1191	L1192	E1195	Y1196		T1209		S1213	P1214		Y1218		L1222	I1223		S1226	GLY			ASP	ALA	ASP	ASN	ARG	GLU	ALA	PRO	HIS	THR <td>ARG</td> <td>LEU</td> <td>GLY</td> <td>GLU</td> <td>LYS</td> <td>ALA</td> <td>LEU</td> <td>ALA</td> <td>TRP</td> <td>ILE</td> <td>ASP</td> <td>SER</td> <td>ASN</td> <td>ALA</td> <td>LYS</td> <td>ALA</td> <td>ASP</td> <td>GLU</td> <td>VAL</td> <td>ILE</td> <td>ASP</td> <td>PRO</td> <td>MET</td> <td>VAL</td> <td>GLY</td> <td>TYR</td> <td>PHE</td>	ARG	LEU	GLY	GLU	LYS	ALA	LEU	ALA	TRP	ILE	ASP	SER	ASN	ALA	LYS	ALA	ASP	GLU	VAL	ILE	ASP	PRO	MET	VAL	GLY	TYR	PHE			
	F1070	V1071		F1074	A1075	H1076	Y1077	Q1078	K1079	L1080		Y1087		S1090		I1097		S1100		I1105		M1108		R1112	L1115		C1129	L1130	M1131	T1132	D1133		I1137	Y1138		D1142		K1146	E1147	I1148	H1149		H1153	A1154	D1155		E1161		Y1165		F1168	K1169	T1170	D1171	Q1172	T1173		V1176	E1177			
	L917		V924		L929		L936	V937		R941		T954		V964	H965		K968	V969		A978		E981	C846	V982	E983		V991		R995	I1001	H1002	F1003	A1004		T1016		M1023		V1028		L1034		R1041		S1048	S1049	S1050	S1051		K1056		M1059	T1060		Y1064	C1065		A1066		A1067		
	T810		V815		E824		T827		M832		V835	Q836	H837	E838	W839		I842	K843	V844	Q845		C846	L847		S850		E853		M864	M865	A866	E867	L868	T869	H870	D871	Q872	D873	C874	H875		R880		R884	Y885	I886		H893	L894	E895	K896		R900		P903	P904		V912	I913	T914		
	R645		M654		M658		L662	E663	N664		T667		L682		A685	D686	K687	Q688	I689	V690		V693		A710		Q714	T715	Y716	I717	T718		K726		Q745		T749		V755		I760	I761	H762	L763	V764	N765	Y766		T767	N768		D771	K772		T784		L792	A628	F629		I796		I805
	V513	F514		F520	H521	T522		H529	E530	G531	R532		L535	T536	G537	R538		M542		I545	N546		Y550	H551	N552	Y553	E554	I555		T567		V575	R576	M577		D583		I586		M600		I606		I610		M614		G615	L616		R620		V624		H627	A628	F629		K636	I637		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.66Å 143.66Å 431.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 3.40 49.11 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.11-3.40) 98.6 (49.11-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472, REFMAC 5.8.0158	Depositor
R, R_{free}	0.228 , 0.275 0.233 , 0.277	Depositor DCC
R_{free} test set	5963 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	141.6	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 123.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	74888	wwPDB-VP
Average B, all atoms (Å ²)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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

5.1 Standard geometry

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

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	0.18	0/9620	0.40	0/13037
1	B	0.18	0/9744	0.40	0/13207
1	C	0.19	0/9706	0.41	0/13153
1	D	0.18	0/9631	0.39	0/13052
All	All	0.18	0/38701	0.40	0/52449

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

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	9403	9210	9210	205	0
1	B	9525	9327	9326	230	0
1	C	9489	9294	9294	212	0
1	D	9414	9217	9217	207	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	D	1	0	0	0	0
All	All	37840	37048	37047	809	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 11.

The worst 5 of 809 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:769:GLN:HB2	1:B:820:ILE:HD13	1.51	0.91
1:C:545:ILE:HD11	1:C:548:LYS:HD2	1.57	0.86
1:C:717:ILE:HD13	1:C:750:LEU:HD22	1.57	0.86
1:C:208:ILE:HB	1:C:232:VAL:HG12	1.56	0.85
1:A:1129:CYS:O	1:A:1132:THR:HG22	1.76	0.85

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	1189/1327 (90%)	1099 (92%)	88 (7%)	2 (0%)	43	71
1	B	1205/1327 (91%)	1105 (92%)	98 (8%)	2 (0%)	43	71
1	C	1199/1327 (90%)	1098 (92%)	101 (8%)	0	100	100
1	D	1189/1327 (90%)	1093 (92%)	94 (8%)	2 (0%)	43	71
All	All	4782/5308 (90%)	4395 (92%)	381 (8%)	6 (0%)	48	78

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1213	SER
1	A	420	SER
1	B	546	ASN
1	B	1157	GLU
1	A	873	ASP

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	1009/1125 (90%)	923 (92%)	86 (8%)	10	33
1	B	1020/1125 (91%)	928 (91%)	92 (9%)	9	30
1	C	1018/1125 (90%)	929 (91%)	89 (9%)	9	32
1	D	1011/1125 (90%)	926 (92%)	85 (8%)	10	34
All	All	4058/4500 (90%)	3706 (91%)	352 (9%)	9	32

5 of 352 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	718	THR
1	D	332	ILE
1	C	865	MET
1	C	1137	ILE
1	D	577	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1185	HIS
1	D	59	HIS
1	D	961	GLN
1	B	402	HIS
1	B	198	HIS

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](#)

Of 9 ligands modelled in this entry, 9 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 [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	1193/1327 (89%)	-0.66	1 (0%) 92 91	96, 218, 342, 403	0
1	B	1209/1327 (91%)	-0.63	1 (0%) 92 91	108, 188, 266, 378	0
1	C	1203/1327 (90%)	-0.62	2 (0%) 91 87	104, 182, 277, 350	0
1	D	1193/1327 (89%)	-0.69	0 100 100	99, 195, 287, 336	0
All	All	4798/5308 (90%)	-0.65	4 (0%) 92 91	96, 190, 308, 403	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1109	LEU	2.7
1	C	386	ALA	2.4
1	C	155	PHE	2.2
1	B	1094	TRP	2.1

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](#)

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
2	CA	A	1401	1/1	0.74	0.15	179,179,179,179	0
3	MG	D	1401	1/1	0.81	0.17	139,139,139,139	0
2	CA	B	1401	1/1	0.86	0.09	154,154,154,154	0
2	CA	B	1402	1/1	0.90	0.12	154,154,154,154	0
2	CA	A	1402	1/1	0.90	0.05	188,188,188,188	0
2	CA	D	1403	1/1	0.91	0.04	172,172,172,172	0
2	CA	C	1401	1/1	0.91	0.07	178,178,178,178	0
2	CA	C	1402	1/1	0.95	0.05	154,154,154,154	0
2	CA	D	1402	1/1	0.98	0.05	129,129,129,129	0

6.5 Other polymers [i](#)

There are no such residues in this entry.