



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 01:37 AM UTC

PDB ID : 5I6I / pdb_00005i6i
Title : Crystal structure of a dBCCP-variant of Chaetomium thermophilum acetyl-CoA carboxylase
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Deposited on : 2016-02-16
Resolution : 8.40 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

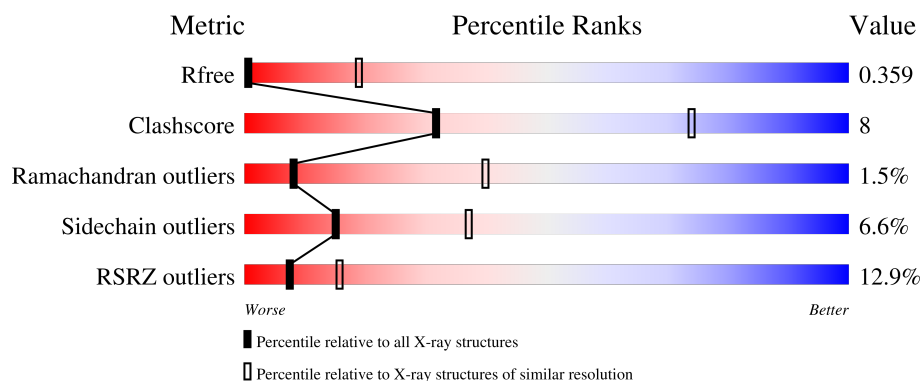
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.40 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	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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	2211	9% 47% 14% • 37%
1	B	2211	8% 48% 14% • 37%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22445 atoms, of which 0 are hydrogens and 0 are deuteriums.

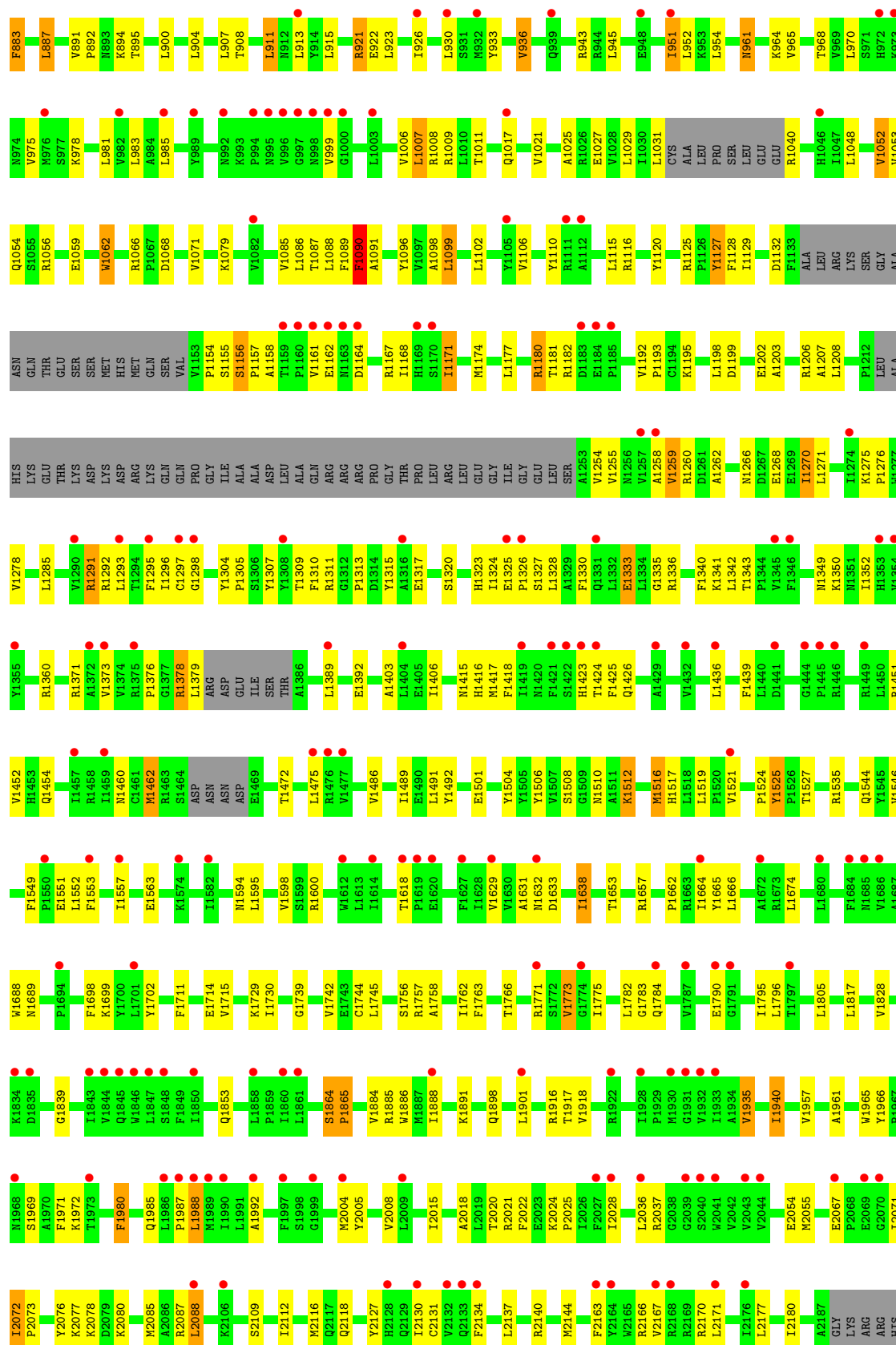
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acetyl-CoA carboxylase-like protein,Acetyl-CoA carboxylase-like protein,Acetyl-CoA carboxylase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1399	Total	C	N	O	S	0	0	0
			11224	7122	1978	2086	38			
1	B	1394	Total	C	N	O	S	0	0	0
			11221	7120	1976	2086	39			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GLY	-	expression tag	UNP G0S3L5
A	763	GLY	-	linker	UNP G0S3L5
A	764	SER	-	linker	UNP G0S3L5
A	765	GLY	-	linker	UNP G0S3L5
B	63	GLY	-	expression tag	UNP G0S3L5
B	763	GLY	-	linker	UNP G0S3L5
B	764	SER	-	linker	UNP G0S3L5
B	765	GLY	-	linker	UNP G0S3L5





UNK	F2163	I2015	R1885	S1766	F1627	L1475	SER	R1292	THR	SER	R1066
UNK	R2166	T2020	W1886	R1757	I1629	R1576	THR	L1293	LYS	THR	P1067
	V2167		I1888	A1758	V1629	V1477		T1294	ASP		D1068
	R2168	K2024	K1891	I1762	A1631	V1486		F1296	ASP		V1071
	R2169	P2025	Q1898	F1763	N1632	I1489		G1298	ARG		
	R2170	I2026		D1633	D1633			R1299	LYS		V1075
	F2027	I2028	L1901	T1766	K1638	Y1492		S1303	GLN		V1076
	E2035	E2036	D1905	R1771	I1638	V1503		Y1307	PRO		T1081
	L2036	R2037	R1916	S1772	V1773	Y1504		F1310	ILE		
	G2038	G2039	T1917	G1774	Y1505	Y1506		P1313	GLY		
	E2054	M2055	V1919	I1775	T1653			Y1315	ALA		L1087
	M2056			Y1778	R1657	M1516		A1316	ALA		L1088
	E2067		I1928	L1782	P1662	H1517		E1317	ASP		F1089
	P2068		P1929	G1783	R1663	H1518		D1319	LEU		F1090
			M1930	Q1784	I1664	L1519		ARG	ALA		A1091
			G1931	Y1665	F1666	F1520		ARG	ALA		H1092
			V1932	L1666		V1521		ARG	ALA		
			I1933			S1522		THR	THR		Y1096
	I2071	I2072	A1934	L1674		T1527		H1323	PRO		
	P2073	P2073	V1935	A1677		W1530		I1324	LEU		L1102
	Y2076		I1940	L1680		L1531		E1325	ARG		E1103
	K2077		Q1956	L1689		Q1532		P1326	ARG		Y1104
	K2078		V1957	N1688		P1533		S1327	GLU		Y1105
	M2085		A1961	F1684		K1534		Q1331	GLY		L1177
	A2086		W1965	N1686		R1535		E1333	ILE		R1107
	R2087		Y1966	A1687		Q1544		L1394	GLY		R1108
	L2088			W1688		Y1545		G1335	GLU		A1109
				N1689		V1546		F1340	LEU		Y1110
	S2109		S1969	F1698		F1549		K1341	SER		L1115
	I2112		A1970	K1699		P1550		P1344			R1116
	M2116		F1971	Y1700		E1551					E1117
	Q2117		K1972	L1701		L1552		Q1348			V1118
	Q2118		Q1985	Y1702		F1553		N1349			R1119
	L2123		L1986	F1711		I1557		K1350			Y1120
	Y2127		F1987	E1714		Q1558		I1352			
	H2128		L1988	V1715		N1559		R1360			F1127
	Q2129		M1989	K1729		E1563		A1372			F1128
	I2130		I1990	I1730		G1579		V1373			I1129
	C2131		A1992	I1731		N1594		V1374			D1130
	Q2133		M1993	T1732		L1595		R1376			W1131
	F2134		R1995	I1733		V1598		P1377			F1133
			R2002	G1739		F1599		ASP			ALA
			M1965	Y1742		R1600		ASN			LEU
	L2137		D1865	E1743		S1606		ASP			LYS
	R2140		D1866	L1745		T1618		ARG			ARG
	S2159		P1867					L1379			LEU
			V1884					L1285			ALA
								V1290			GLN
								THR			THR
								GLY			GLY
								ALA			ALA
								ASN			ASN
								GLN			GLN
								THR			THR
								LYS			LYS
								GLU			GLU
								SER			SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	462.20Å 462.20Å 204.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.95 – 8.40 49.95 – 8.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.95-8.40) 99.0 (49.95-8.40)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 8.33Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.297 , 0.324 0.338 , 0.359	Depositor DCC
R_{free} test set	549 reflections (3.25%)	wwPDB-VP
Wilson B-factor (Å ²)	572.4	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 973.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	22445	wwPDB-VP
Average B, all atoms (Å ²)	250.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% 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	0.76	2/11401 (0.0%)	1.32	39/15435 (0.3%)
1	B	0.75	1/11458 (0.0%)	1.31	35/15511 (0.2%)
All	All	0.75	3/22859 (0.0%)	1.32	74/30946 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2224	THR	CA-C	5.92	1.57	1.53
1	B	2072	ILE	CA-C	5.21	1.58	1.52
1	A	2072	ILE	CA-C	5.08	1.58	1.52

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1090	PHE	CA-CB-CG	6.40	120.20	113.80
1	B	1090	PHE	CA-CB-CG	6.38	120.18	113.80
1	B	853	PRO	CA-C-N	6.37	129.45	120.28
1	B	853	PRO	C-N-CA	6.37	129.45	120.28
1	A	853	PRO	CA-C-N	6.34	129.41	120.28

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	11224	0	11148	187	0
1	B	11221	0	11191	181	0
All	All	22445	0	22339	363	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 8.

The worst 5 of 363 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:1192:VAL:HG21	1:A:1203:ALA:HB1	1.48	0.94
1:B:1108:ARG:HH21	1:B:1375:ARG:HH22	1.21	0.85
1:B:1864:SER:HB2	1:B:1865:PRO:HD3	1.65	0.79
1:B:2054:GLU:HG3	1:B:2203:PRO:HG2	1.65	0.79
1:A:1864:SER:HB2	1:A:1865:PRO:HD3	1.65	0.78

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	1373/2211 (62%)	1229 (90%)	123 (9%)	21 (2%)	8	40
1	B	1380/2211 (62%)	1249 (90%)	110 (8%)	21 (2%)	8	40
All	All	2753/4422 (62%)	2478 (90%)	233 (8%)	42 (2%)	8	40

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	943	ARG
1	A	1156	SER
1	A	1516	MET

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Mol	Chain	Res	Type
1	A	1784	GLN
1	A	1864	SER

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	1208/1879 (64%)	1127 (93%)	81 (7%)	15	36
1	B	1215/1879 (65%)	1137 (94%)	78 (6%)	16	37
All	All	2423/3758 (64%)	2264 (93%)	159 (7%)	15	37

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1198	LEU
1	B	1817	LEU
1	B	1327	SER
1	B	1595	LEU
1	B	1957	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	957	GLN
1	B	1460	ASN
1	B	992	ASN
1	B	1415	ASN
1	B	1481	ASN

5.3.3 RNA ⓘ

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	1387/2211 (62%)	0.53	189 (13%)	7 15	25, 211, 483, 500	0
1	B	1394/2211 (63%)	0.51	169 (12%)	8 17	5, 245, 486, 500	0
All	All	2781/4422 (62%)	0.52	358 (12%)	7 16	5, 230, 485, 500	0

The worst 5 of 358 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1862	SER	20.1
1	A	792	VAL	17.5
1	B	1796	LEU	16.4
1	B	1389	LEU	11.3
1	A	2069	GLU	11.2

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.