



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 02:42 AM UTC

PDB ID : 5CSK / pdb_00005csk
Title : Crystal structure of yeast acetyl-CoA carboxylase, unbiotinylated
Authors : Wei, J.; Tong, L.
Deposited on : 2015-07-23
Resolution : 3.10 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

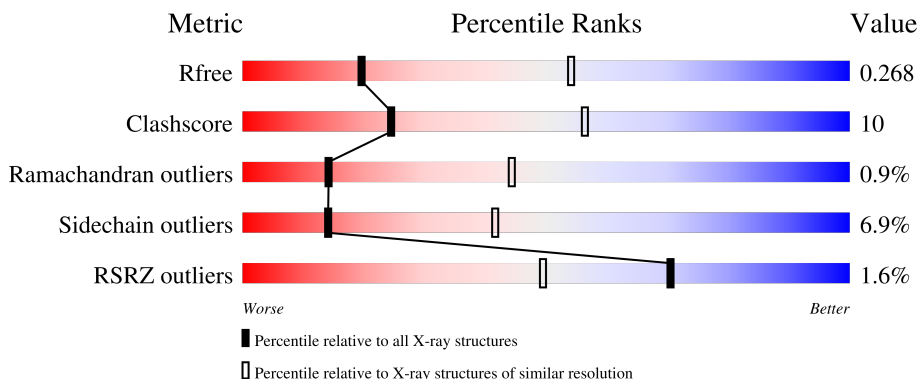
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	2218	66% 22% • 10%
1	B	2218	2% 67% 21% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31806 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1996	Total	C	N	O	S	0	0	0
			15828	10063	2733	2980	52			
1	B	2017	Total	C	N	O	S	0	0	0
			15978	10159	2758	3009	52			

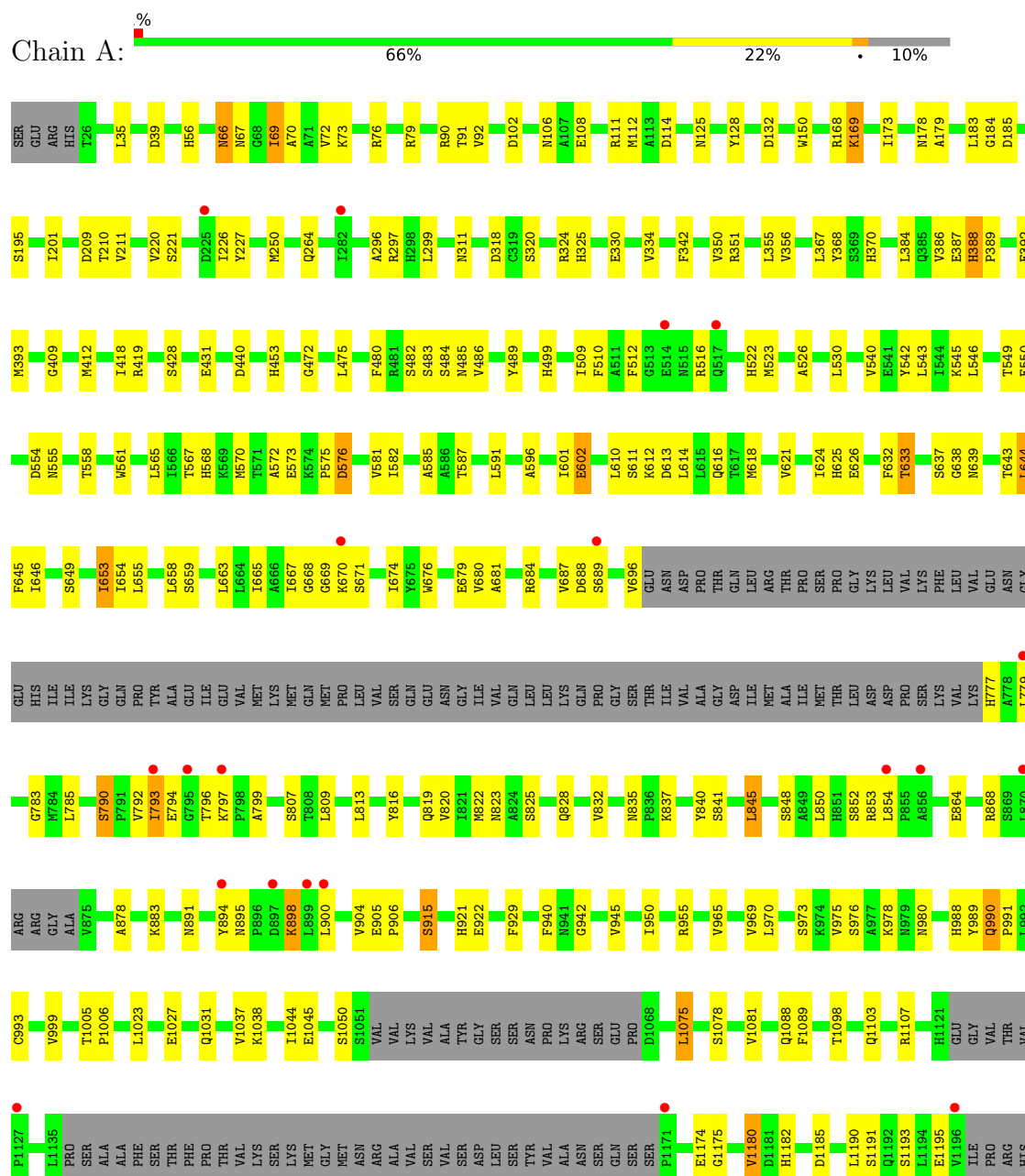
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2234	HIS	-	expression tag	UNP Q00955
A	2235	HIS	-	expression tag	UNP Q00955
A	2236	HIS	-	expression tag	UNP Q00955
A	2237	HIS	-	expression tag	UNP Q00955
A	2238	HIS	-	expression tag	UNP Q00955
A	2239	HIS	-	expression tag	UNP Q00955
B	2234	HIS	-	expression tag	UNP Q00955
B	2235	HIS	-	expression tag	UNP Q00955
B	2236	HIS	-	expression tag	UNP Q00955
B	2237	HIS	-	expression tag	UNP Q00955
B	2238	HIS	-	expression tag	UNP Q00955
B	2239	HIS	-	expression tag	UNP Q00955

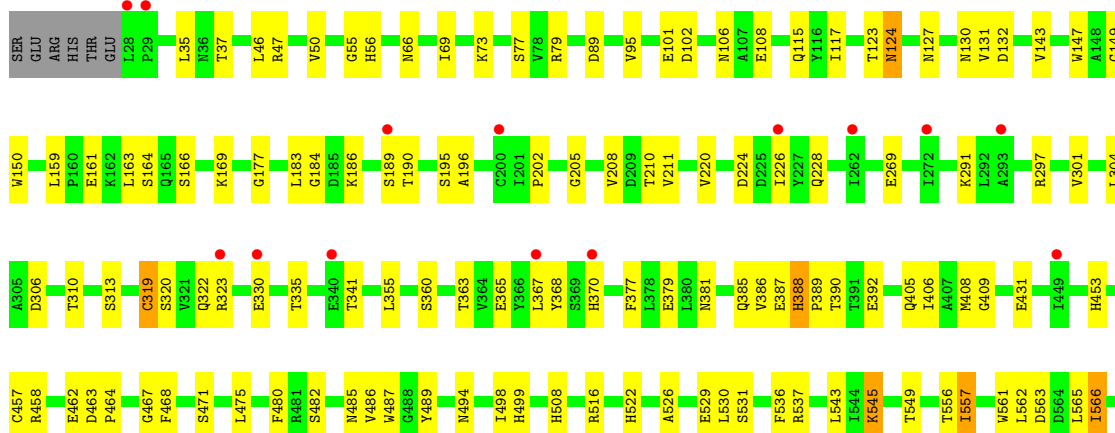
3 Residue-property plots [i](#)

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: Acetyl-CoA carboxylase



- Molecule 1: Acetyl-CoA carboxylase



R2080	E2081	L2082	L2083	P2084	L2085	Y2086	I2089	S2101	R2102	M2103	K2106	W2115	T2116	E2117	A2118	R2128	N2131	R2138	H2141	GLN	VAL	GLY	GLU	A2146	I2152	S2162	Y2163	D2164	H2165	D2168	R2169	Q2170	W2174	I2175	E2176	E2177	W2178	T2179	L2180	L2181	L2182	D2183	L2186	L2189	K2190		
T1792	L1797	K1802	M1807	S1808	Y1809	V1810	K1813	V1818	T1823	K1824	D1825	T1826	W1827	D1828	R1829	P1830	F1833	T1836	N1837	D1838	E1839	T1840	Y1841	R1842	M1846	G1849	T1852	G1855	Y1858	A1874	K1875	V1878	R1883	I1887	P1888	V1894	N1909	E2079									
E1914	T1915	P1920	V1923	W1924	H1925	P1926	S1927	E1943	Q1944	L1945	S1957	Q1960	R1961	D1962	M1963	F1964	D1980	Y1988	P1991	T1992	V2001	A2022	G2023	V2024	L2025	E2026	P2027	V2031	G2032	I2033	K2034	F2035	R2036	S2059	ASN	LYS	SER	LEU	ALA	PRO	GLU	VAL	R2068				
T1692	E1703	C1704	L1705	A1714	Y1719	T1724	I1725	C1730	R1731	S1732	I1735	K1736	A1737	L1739	V1740	R1741	L1742	G1743	Q1744	R1745	Q1748	G1751	Q1752	A1759	P1760	A1761	I1762	M1763	K1764	M1765	L1766	E1769	V1770	Y1771	N1774	L1775	Q1776	L1777	Q1781	I1782	ALA	M1783	N1786	G1787	V1788	S1789	
V1584	W1585	I1589	K1592	I1593	G1594	F1603	F1604	N1605	K1606	V1607	I1616	I1619	A1632	E1633	E1634	I1635	V1636	P1637	L1638	F1639	V1641	A1642	W1643	N1648	P1649	D1650	K1651	G1652	F1653	Q1654	Y1655	L1656	Y1657	L1658	E1664	T1665	K1667	D1670	T1680	V1681	V1671	N1682	N1683	F1688	V1689	I1690	K1691
V1468	F1469	S1471	S1477	W1478	H1479	L1480	Y1487	K1490	E1491	W1492	L1493	R1497	Y1498	K1499	T1506	Y1507	V1508	Q1517	S1521	T1533	D1534	F1537	I1538	S1539	L1542	T1543	E1544	E1549	L1550	P1557	G1558	V1565	A1566	F1567	K1568	I1569	T1570	V1571	T1572	T1573	R1580	Q1581	F1582	V1583			
T1344	D1350	I1351	S1352	I1353	S1359	L1364	M1365	T1368	L1369	N1371	V1374	T1375	D1376	S1380	T1385	N1388	F1389	I1390	F1393	G1406	F1407	L1408	E1409	L1415	S1422	K1430	T1434	P1437	R1441	T1444	N1445	V1451	T1454	V1460	K1461	E1466	W1467										
V1468	F1469	S1471	S1477	W1478	H1479	L1480	Y1487	K1490	E1491	W1492	L1493	R1497	Y1498	K1499	T1506	Y1507	V1508	Q1517	S1521	T1533	D1534	F1537	I1538	S1539	L1542	T1543	E1544	E1549	L1550	P1557	G1558	V1565	A1566	F1567	K1568	I1569	T1570	V1571	T1572	T1573	R1580	Q1581	F1582	V1583			
V1584	W1585	I1589	K1592	I1593	G1594	F1603	F1604	N1605	K1606	V1607	I1616	I1619	A1632	E1633	E1634	I1635	V1636	P1637	L1638	F1639	V1641	A1642	W1643	N1648	P1649	D1650	K1651	G1652	F1653	Q1654	Y1655	L1656	Y1657	L1658	E1664	T1665	K1667	D1670	T1680	V1681	V1671	N1682	N1683	F1688	V1689	I1690	K1691
T1692	E1703	C1704	L1705	A1714	Y1719	T1724	I1725	C1730	R1731	S1732	I1735	K1736	A1737	L1739	V1740	R1741	L1742	G1743	Q1744	R1745	Q1748	G1751	Q1752	A1759	P1760	A1761	I1762	M1763	K1764	M1765	L1766	E1769	V1770	Y1771	N1774	L1775	Q1776	L1777	Q1781	I1782	ALA	M1783	N1786	G1787	V1788	S1789	
T1792	L1797	K1802	M1807	S1808	Y1809	V1810	K1813	V1818	T1823	K1824	D1825	T1826	W1827	D1828	R1829	P1830	F1833	T1836	N1837	D1838	E1839	T1840	Y1841	R1842	M1846	G1849	T1852	G1855	Y1858	A1874	K1875	V1878	R1883	I1887	P1888	V1894	N1909	E2079									
E1914	T1915	P1920	V1923	W1924	H1925	P1926	S1927	E1943	Q1944	L1945	S1957	Q1960	R1961	D1962	M1963	F1964	D1980	Y1988	P1991	T1992	V2001	A2022	G2023	V2024	L2025	E2026	P2027	V2031	G2032	I2033	K2034	F2035	R2036	S2059	ASN	LYS	SER	LEU	ALA	PRO	GLU	VAL	R2068				
R2080	E2081	L2082	L2083	P2084	L2085	Y2086	I2089	S2101	R2102	M2103	K2106	W2115	T2116	E2117	A2118	R2128	N2131	R2138	H2141	GLN	VAL	GLY	GLU	A2146	I2152	S2162	Y2163	D2164	H2165	D2168	R2169	Q2170	W2174	I2175	E2176	E2177	W2178	T2179	L2180	L2181	L2182	D2183	L2186	L2189	K2190		
L854	L865	R868	S869	L870	ARG	ARG	GLY	A874	V875	F876	F877	A878	K883	D886	D887	K888	L889	L900	V904	E905	GLN	P906	K913	Y914	H921	E922	H923	S924	Y925	F926	V927	H928	Y933	F940	N941	V945	P950	R955	L967	V975	N979	N980	L981				
Q990	P991	S997	P1006	V1011	E1012	L1013	E1014	S1015	R1026	L1030	R1040	I1044	V1052	V1053	Y1057	G1058	SER	ASN	PRO	LYS	ARG	S1065	L1075	S1078	V1081	D1084	P1095	T1098	A1099	Q1103	R1108	E1122	GLY	VAL	THR	VAL	P1127	I1128									
L1135	P1136	S1137	ALA	PHE	SER	THR	PHE	THR	VAL	LYS	SER	LYS	MET	ASN	R1154	S1162	T1162	VAL	ALA	ASN	SER	GLN	SER	S1170	G1175	I1176	M1177	A1179	V1180	D1185	V1186	D1187	L1190	S1191	I1197	PRO	ARG	HIS	GLN	SER	SER	ASN	GLY	PRO	ALA	ASP	ARG
Q990	P991	S997	P1006	V1011	E1012	L1013	E1014	S1015	R1026	L1030	R1040	I1044	V1052	V1053	Y1057	G1058	SER	ASN	PRO	LYS	ARG	S1065	L1075	S1078	V1081	D1084	P1095	T1098	A1099	Q1103	R1108	E1122	GLY	VAL	THR	VAL	P1127	I1128									
L1135	P1136	S1137	ALA	PHE	SER	THR	PHE	THR	VAL	LYS	SER	LYS	MET	ASN	R1154	S1162	T1162	VAL	ALA	ASN	SER	GLN	SER	S1170	G1175	I1176	M1177	A1179	V1180	D1185	V1186	D1187	L1190	S1191	I1197	PRO	ARG	HIS	GLN	SER	SER	ASN	GLY	PRO	ALA	ASP	ARG
Q990	P991	S997	P1006	V1011	E1012	L1013	E1014	S1015	R1026	L1030	R1040	I1044	V1052	V1053	Y1057	G1058	SER	ASN	PRO	LYS	ARG	S1065	L1075	S1078	V1081	D1084	P1095	T1098	A1099	Q1103	R1108	E1122	GLY	VAL	THR	VAL	P1127	I1128									
L1135	P1136	S1137	ALA	PHE	SER	THR	PHE	THR	VAL	LYS	SER	LYS	MET	ASN	R1154	S1162	T1162	VAL	ALA	ASN	SER	GLN	SER	S1170	G1175	I1176	M1177	A1179	V1180	D1185	V1186	D1187	L1190	S1191	I1197	PRO	ARG	HIS	GLN	SER	SER	ASN	GLY	PRO	ALA	ASP	ARG
Q990	P991	S997	P1006	V1011	E1012	L1013	E1014	S1015	R1026	L1030	R1040	I1044	V1052	V1053	Y1057	G1058	SER	ASN	PRO	LYS	ARG	S1065	L1075	S1078	V1081	D1084	P1095	T1098	A1099	Q1103	R1108	E1122	GLY	VAL	THR	VAL	P1127	I1128									
L1135	P1136	S1137	ALA	PHE	SER	THR	PHE	THR	VAL	LYS	SER	LYS	MET	ASN	R1154	S1162	T1162	VAL	ALA	ASN	SER	GLN	SER	S1170	G1175	I1176	M1177	A1179	V1180	D1185	V1186	D1187	L1190	S1191	I1197	PRO	ARG	HIS	GLN	SER	SER	ASN	GLY	PRO	ALA	ASP	ARG
Q990	P991	S997	P1006	V1011	E1012	L1013	E1014	S1015	R1026	L1030	R1040	I1044	V1052	V1053	Y1057	G1058	SER	ASN	PRO	LYS	ARG	S1065	L1075	S1078	V1081	D1084	P1095	T1098	A1099	Q1103	R1108	E1122	GLY	VAL	THR	VAL	P1127	I1128									
L1135	P1136	S1137	ALA	PHE	SER	THR	PHE	THR	VAL	LYS	SER	LYS	MET	ASN	R1154	S1162	T1162	VAL	ALA	ASN	SER	GLN	SER	S1170	G1175	I1176	M1177	A1179	V1180	D1185	V1186	D1187	L1190	S1191	I1197	PRO	ARG	HIS	GLN	SER	SER	ASN	GLY	PRO	ALA	ASP	ARG
Q990	P991	S997	P1006	V1011	E1012	L1013	E1014	S1015	R1026	L1030	R1040	I1044	V1052	V1053	Y1057	G1058	SER	ASN	PRO	LYS	ARG	S1065	L1075	S1078	V1081	D1084	P1095	T1098	A1099	Q1103	R1108	E1122	GLY	VAL	THR	VAL	P1127	I1128									
L1135	P1136	S1137	ALA	PHE	SER	THR	PHE	THR	VAL	LYS	SER	LYS	MET	ASN	R1154	S1162	T1162	VAL	ALA	ASN	SER	GLN	SER	S1170	G1175	I1176	M1177	A1179	V1180	D1185	V1186	D1187	L1190	S1191	I1197	PRO	ARG	HIS	GLN	SER	SER	ASN	GLY	PRO	ALA	ASP	ARG
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L1135	P1136	S1137	ALA	PHE	SER	THR	PHE	THR	VAL	LYS	SER	LYS	MET	ASN	R1154	S1162	T1162	VAL	ALA	ASN	SER	GLN	SER	S1170	G1175	I1176	M1177	A1179	V1180	D1185	V1186	D1187	L1190	S1191	I1197	PRO	ARG	HIS	GLN	SER	SER	ASN	GLY	PRO	ALA	ASP	ARG
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L1135	P1136	S1137	ALA	PHE	SER	THR	PHE	THR	VAL	LYS	SER	LYS	MET	ASN	R1154	S1162	T1162	VAL	ALA	ASN	SER	GLN	SER	S1170	G1175	I1176	M1177	A1179	V1180	D1185	V1186	D1187	L1190	S1191	I1197	PRO	ARG	HIS	GLN	SER	SER	ASN	GLY	PRO	ALA	ASP	ARG
Q990	P991	S997	P1006	V1011	E1012	L1013	E1014	S1015	R1026	L1030	R1040	I1044	V1052	V1053	Y1057	G1058	SER	ASN	PRO	LYS	ARG	S1065	L1075	S1078	V1081	D1084	P1095	T1098	A1099	Q1103	R1108	E1122	GLY	VAL	THR	VAL	P1127	I1128									
L1135	P1136	S1137	ALA	PHE	SER	THR	PHE	THR	VAL	LYS	SER	LYS	MET	ASN	R1154	S1162	T1162	VAL	ALA	ASN	SER	GLN	SER	S1170	G1175	I1176	M1177	A1179	V1180	D1185	V1186	D1187	L1190	S1191	I1197	PRO	ARG	HIS	GLN	SER	SER	ASN	GLY	PRO	ALA	ASP	ARG
Q990	P991	S997	P1006	V1011	E1012	L1013	E1014	S1015	R1026	L1030	R1040	I1044	V1052	V1053	Y1057	G1058	SER	ASN	PRO	LYS	ARG	S1065	L1075	S1078	V1081	D1084	P1095	T1098	A1099	Q1103	R1108	E1122	GLY	VAL	THR	VAL	P1127	I1128									
L1135	P1136	S1137	ALA	PHE	SER	THR	PHE	THR	VAL	LYS	SER	LYS	MET	ASN	R1154	S1162	T1162	VAL	ALA	ASN	SER	GLN	SER	S1																							

L2191	
E2192	
S2193	
PHE	
ALA	
GLN	
ASP	
LEU	
ALA	
LYS	
LYS	
ILE	
ARG	
SER	
ASP	
HIS	
ASP	
ASN	
ALA	
ILE	
ASP	
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ILE	
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SER	
THR	
ASP	
ASP	
LYS	
GLU	
LYS	
LEU	
LEU	
LYS	
THR	
LEU	
LYS	
HIS	
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4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.88Å 159.88Å 615.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 3.10 49.47 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.0 (49.47-3.10) 93.3 (49.47-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.217 , 0.281 (Not available) , 0.268	Depositor DCC
R_{free} test set	6831 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	85.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.3	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	0.93	EDS
Total number of atoms	31806	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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	0.77	1/16156 (0.0%)	1.02	34/21869 (0.2%)
1	B	0.77	1/16306 (0.0%)	1.02	32/22069 (0.1%)
All	All	0.77	2/32462 (0.0%)	1.02	66/43938 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1592	LYS	CA-C	-8.65	1.47	1.52
1	B	1573	THR	N-CA	5.40	1.49	1.46

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1990	PRO	CA-C-N	7.51	129.23	119.84
1	A	1990	PRO	C-N-CA	7.51	129.23	119.84
1	A	1174	GLU	N-CA-C	6.72	118.42	108.60
1	B	1571	VAL	CB-CA-C	-6.65	100.27	110.50
1	A	1434	THR	N-CA-C	6.60	118.56	111.36

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	15828	0	15783	316	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	15978	0	15941	344	0
All	All	31806	0	31724	630	1

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 10.

The worst 5 of 630 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:1841:TYR:CE1	1:A:1846:MET:HE3	1.87	1.10
1:A:1835:PRO:HG3	1:A:1846:MET:HE2	1.30	1.09
1:A:1735:ILE:HD13	1:A:1735:ILE:H	1.19	1.07
1:B:941:ASN:HD21	1:B:1013:LEU:HA	1.31	0.92
1:B:1040:ARG:NH1	1:B:1081:VAL:O	2.02	0.92

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ASP:OD1	1:A:440:ASP:OD1[7_466]	1.80	0.40

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	1980/2218 (89%)	1771 (89%)	188 (10%)	21 (1%)	11	39
1	B	1997/2218 (90%)	1778 (89%)	203 (10%)	16 (1%)	16	47
All	All	3977/4436 (90%)	3549 (89%)	391 (10%)	37 (1%)	14	44

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	572	ALA
1	A	184	GLY
1	A	573	GLU
1	A	1316	ASP
1	A	1378	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	1323/1912 (69%)	1223 (92%)	100 (8%)	12	39
1	B	1735/1912 (91%)	1624 (94%)	111 (6%)	16	44
All	All	3058/3824 (80%)	2847 (93%)	211 (7%)	14	41

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	557	ILE
1	B	1190	LEU
1	B	1915	THR
1	B	653	ILE
1	B	886	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1384	HIS
1	B	1941	ASN
1	B	1522	GLN
1	B	1781	GLN
1	B	2057	GLN

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	1996/2218 (89%)	-0.06	32 (1%)	70 49	47, 85, 140, 237	0
1	B	2017/2218 (90%)	-0.02	34 (1%)	69 48	46, 87, 161, 237	0
All	All	4013/4436 (90%)	-0.04	66 (1%)	70 49	46, 86, 150, 237	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	945	VAL	5.5
1	B	1197	ILE	3.9
1	A	856	ALA	3.7
1	B	2182	LEU	3.4
1	B	794	GLU	3.3

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.