



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:41 PM UTC

PDB ID : 5I6H / pdb_00005i6h
Title : Crystal structure of CD-CT domains of Chaetomium thermophilum acetyl-CoA carboxylase
Authors : Hunkeler, M.; Stuttfeld, E.; Hagmann, A.; Imseng, S.; Maier, T.
Deposited on : 2016-02-16
Resolution : 7.20 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

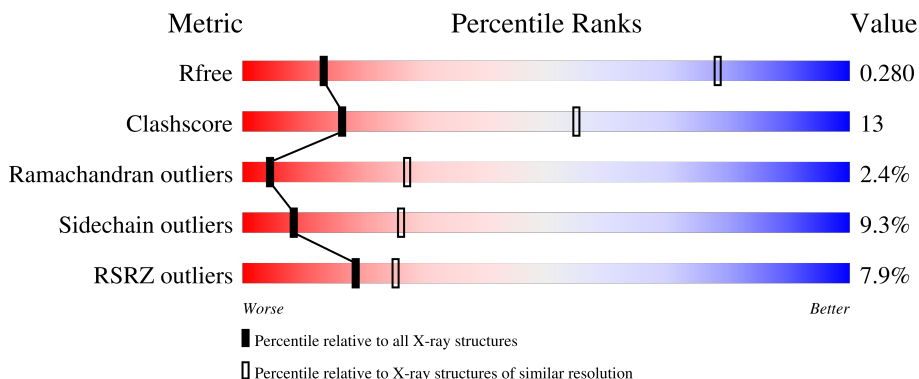
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.20 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	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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	1487	7% 60% 29% 6%
1	B	1487	8% 61% 29% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22543 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.

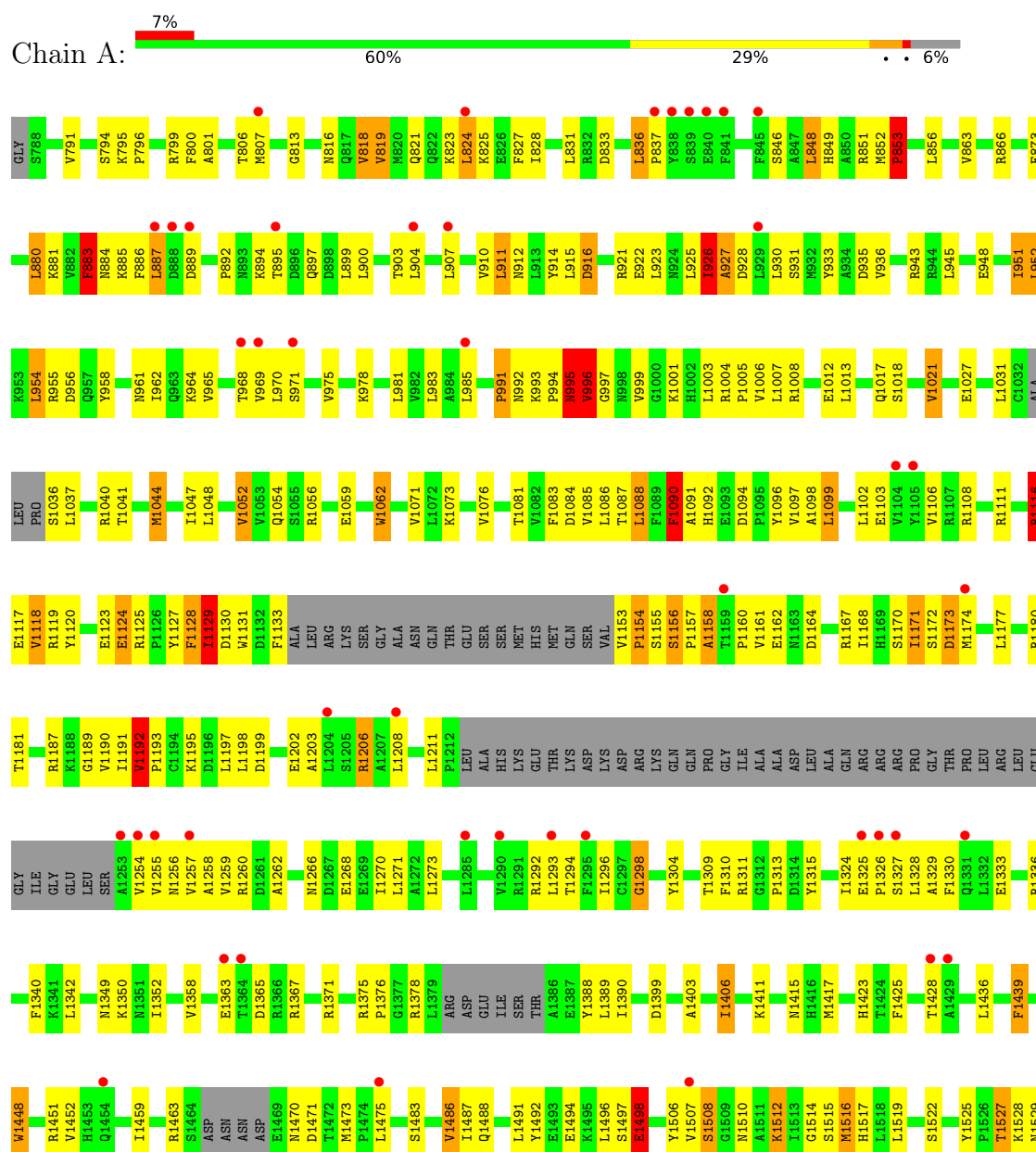
- Molecule 1 is a protein called Acetyl-CoA carboxylase-like protein.

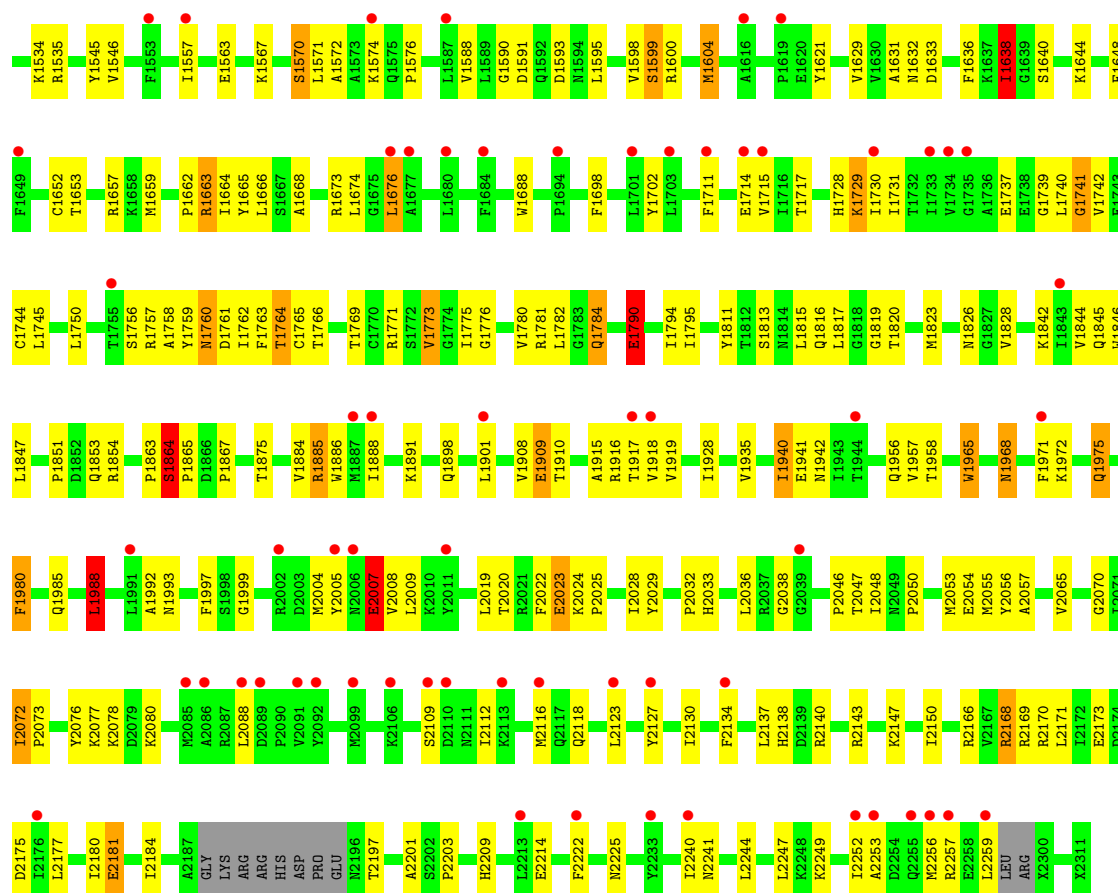
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1404	Total	C	N	O	S	0	0	0
			11262	7144	1983	2096	39			
1	B	1406	Total	C	N	O	S	0	0	0
			11281	7156	1988	2098	39			

3 Residue-property plots

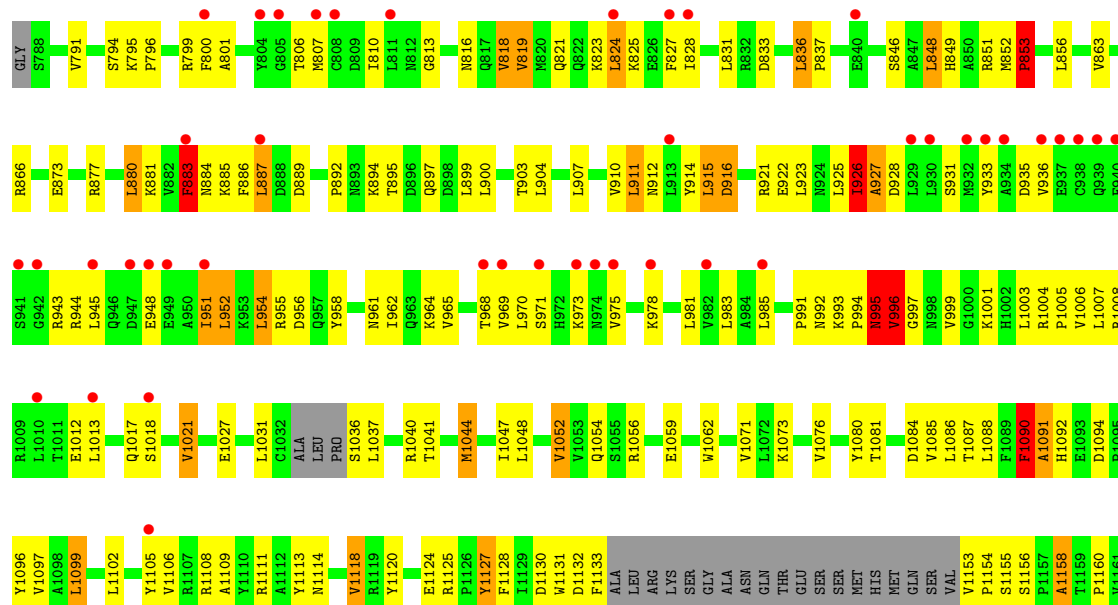
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-like protein





• Molecule 1: Acetyl-CoA carboxylase-like protein



K2243	L2036	P1945	V1828	H1728	V1630	I1513	V1432	H1323	ALA	E1162
L2244	R2037	E1955	S1829	K1729	A1631	G1514	A1433	I1324	ALA	N1163
E2245	G2038	Q1956	H1830	I1730	I1731	S1515	S1434	E1325	ASP	D1164
K2246	G2039	V1957	K1842	T1732	D1633	H1517	L1436	P1326	LEU	R1167
K2249	P2046	T1958	I1843	I1733	F1636	L1518	F1439	S1327	ALA	I1168
	T2047	W1965	V1844	E1737	K1637	L1519	W1448	L1328	ARG	I1171
	I2048	Q1845	Q1845	E1738	P1637	P1520	W1448	L1332	ARG	S1172
	M2049	L1847	V1846	G1739	G1639	S1522	W1448	E1333	PRO	D1173
	P2050	L1847	L1847	L1740	S1640	S1522	R1451	L1334	GLY	M1174
	M2053	F1971	P1851	G1741	K1644	Y1526	H1452	G1335	THR	T1175
	E2054	K1972	D1852	V1742	F1648	T1527	H1452	R1336	PRO	Y1176
	M2055	Q1853	Q1853	E1743	F1648	K1528	Q1454	L1336	LEU	L1177
	Y2056	R1854	R1854	L1744	F1649	N1529	N1460	F1340	ARG	R1180
	A2057	L1858	L1858	L1745	F1649	W1530	M1462	P1344	LEU	T1181
	V2065	L1858	L1858	L1750	C1652	W1530	M1462	P1344	GLY	R1182
	L2066	L1861	L1861	L1756	T1653	P1533	R1463	M1349	ILE	R1187
	E2067	S1862	S1862	S1756	R1657	K1534	S1464	I1352	GLY	K1188
	P2068	P1863	P1863	R1757	K1658	R1535	ASP	H1353	LEU	G1189
	E2069	S1864	S1864	A1758	M1659	Y1545	ASN	V1354	SER	V1190
	G2070	P1865	P1865	Y1759	G1660	V1546	ASN	Y1355	LEU	I1191
	I2071	L1866	L1866	D1760	G1661	Y1546	ASP	F1369	ASP	V1192
	I2072	P1867	P1867	N1761	P1662	I1557	E1469	T1370	LEU	P1193
	P2073	P1867	P1867	L1762	P1662	I1557	E1469	K1194	LEU	C1195
	Y2076	T1875	T1875	F1763	Y1665	E1563	M1473	R1260	GLY	D1196
	K2077	V1884	V1884	T1766	L1666	A1564	P1474	D1261	LEU	L1197
	K2078	P1885	P1885	T1766	S1667	A1564	R1476	L1262	GLY	L1198
	D2079	W1886	W1886	G1770	A1668	K1567	I1477	E1263	LEU	E1202
	K2080	W1887	W1887	T1769	Y1665	E1563	I1478	L1265	ASP	L1203
	T2084	I1888	I1888	R1771	L1673	A1564	I1479	L1206	GLY	S1205
	M2085	S1772	S1772	L1674	L1674	L1571	T1480	L1208	LEU	A1207
	K2086	G1773	G1773	G1675	G1675	A1572	N1481	E1209	LEU	L1210
	L2088	L1775	L1775	L1676	L1676	K1574	T1482	P1212	LEU	L1211
	D2089	G1776	G1776	L1680	L1680	P1576	S1483	R1291	LEU	P1212
	Y2092	L1901	L1901	V1780	H1683	P1576	V1486	L1292	ALA	LEU
	S2109	V1908	V1908	R1781	F1684	V1588	Q1488	L1285	HIS	ALA
	L2112	T1910	T1910	L1782	M1685	L1489	I1489	L1285	GLY	HIS
	K2113	L1911	L1911	G1783	V1686	D1593	E1491	R1291	GLY	GLY
	M2116	A1915	A1915	Q1784	A1687	L1595	Y1492	L1292	THR	THR
	Q2117	R1916	R1916	E1790	W1688	A1596	E1493	L1293	LYS	LYS
	R2118	T1917	T1917	I1795	P1694	V1598	E1494	F1294	LYS	LYS
	R2119	V1918	V1918	I1795	P1694	S1599	K1495	F1295	GLY	GLY
	E2120	V1919	V1919	P1698	F1698	R1600	L1496	G1298	LYS	LYS
	L2123	I1928	I1928	S1813	L1701	E1601	W1502	Y1307	ASP	ASP
	L2123	P2025	P2025	M1814	Y1702	P1602	V1503	F1310	LYS	LYS
	Y2127	V1935	V1935	Q1816	F1711	G1603	Y1505	R1311	ARG	ARG
	Y2127	V1935	V1935	L1817	F1711	M1604	Y1505	G1312	LYS	LYS
	L2130	T1940	T1940	G1818	E1714	M1609	Y1506	H1423	GLN	GLN
	Q2133	E1941	E1941	G1819	V1715	P1619	S1508	D1314	PRO	PRO
	F2134	N1942	N1942	T1820	T1716	E1620	N1510	Y1315	GLY	GLY
		I1943	I1943	N1826	T1717	Y1621		D1319	ILE	ILE
		T1944	T1944	G1827						

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	295.02Å 295.02Å 189.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.85 – 7.20 49.85 – 7.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.85-7.20) 99.6 (49.85-7.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 7.37Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.232 , 0.248 0.261 , 0.280	Depositor DCC
R_{free} test set	696 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	662.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 928.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	22543	wwPDB-VP
Average B, all atoms (Å ²)	271.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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	0.85	7/11439 (0.1%)	1.40	80/15486 (0.5%)
1	B	0.85	6/11458 (0.1%)	1.40	75/15511 (0.5%)
All	All	0.85	13/22897 (0.1%)	1.40	155/30997 (0.5%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	926	ILE	CA-C	8.10	1.63	1.52
1	A	926	ILE	CA-C	7.88	1.62	1.52
1	A	1988	LEU	CA-C	-6.82	1.44	1.52
1	A	2072	ILE	CA-CB	6.33	1.57	1.54
1	B	1988	LEU	CA-C	-6.10	1.45	1.52

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1261	ASP	CA-CB-CG	9.71	122.31	112.60
1	B	1090	PHE	CA-CB-CG	8.53	122.33	113.80
1	A	1090	PHE	CA-CB-CG	8.13	121.93	113.80
1	B	1980	PHE	CA-CB-CG	8.04	121.84	113.80
1	A	883	PHE	CA-CB-CG	7.76	121.56	113.80

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	11262	0	11181	295	0
1	B	11281	0	11205	300	0
All	All	22543	0	22386	582	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 582 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:1389:LEU:HD11	1:B:1425:PHE:HB3	1.33	1.08
1:A:994:PRO:HA	1:A:1037:LEU:HB3	1.35	1.07
1:B:1609:MET:HE1	1:B:1630:VAL:HG13	1.33	1.04
1:B:994:PRO:HA	1:B:1037:LEU:HB3	1.40	1.01
1:A:1090:PHE:HB2	1:A:1193:PRO:HB3	1.39	0.99

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	1378/1487 (93%)	1221 (89%)	121 (9%)	36 (3%)	4	25
1	B	1380/1487 (93%)	1221 (88%)	130 (9%)	29 (2%)	5	30
All	All	2758/2974 (93%)	2442 (88%)	251 (9%)	65 (2%)	4	27

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	819	VAL
1	A	943	ARG
1	A	1092	HIS

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Mol	Chain	Res	Type
1	A	1117	GLU
1	A	1128	PHE

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	1213/1282 (95%)	1099 (91%)	114 (9%)	8	25
1	B	1215/1282 (95%)	1104 (91%)	111 (9%)	9	27
All	All	2428/2564 (95%)	2203 (91%)	225 (9%)	8	26

5 of 225 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	816	ASN
1	B	2197	THR
1	B	1090	PHE
1	B	2171	LEU
1	B	1901	LEU

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	B	2049	ASN
1	B	2129	GLN
1	B	2212	GLN
1	A	2049	ASN
1	A	1985	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2261:ARG	C	2300:UNK	N	9.73

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	1392/1487 (93%)	0.21	106 (7%)	20 26	33, 251, 497, 500	0
1	B	1394/1487 (93%)	0.23	115 (8%)	17 25	13, 262, 498, 500	0
All	All	2786/2974 (93%)	0.22	221 (7%)	18 25	13, 258, 497, 500	0

The worst 5 of 221 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	933	TYR	14.2
1	A	2256	MET	10.8
1	B	2256	MET	9.9
1	A	2092	TYR	8.4
1	A	2088	LEU	8.4

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.