



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:07 AM GMT

PDB ID : 2VZ8  
Title : CRYSTAL STRUCTURE OF MAMMALIAN FATTY ACID SYNTHASE  
Authors : Maier, T.; Leibundgut, M.; Ban, N.  
Deposited on : 2008-07-31  
Resolution : 3.22 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

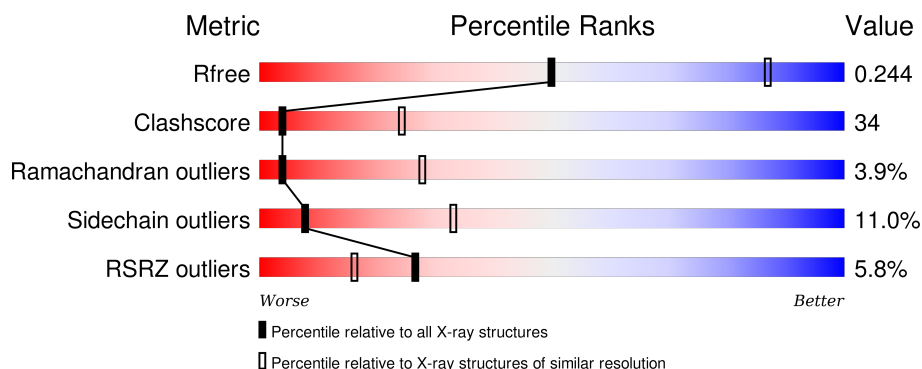
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.22 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))
$R_{free}$	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	2512	<div> <div>4%</div> <div>35%</div> <div>36%</div> <div>6%</div> <div>22%</div> </div>
1	B	2512	<div> <div>6%</div> <div>36%</div> <div>37%</div> <div>6%</div> <div>20%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30281 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 FATTY ACID SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1962	Total	C	N	O	S	0	0	0
			14977	9466	2630	2803	78			
1	B	2004	Total	C	N	O	S	0	0	0
			15304	9671	2684	2869	80			

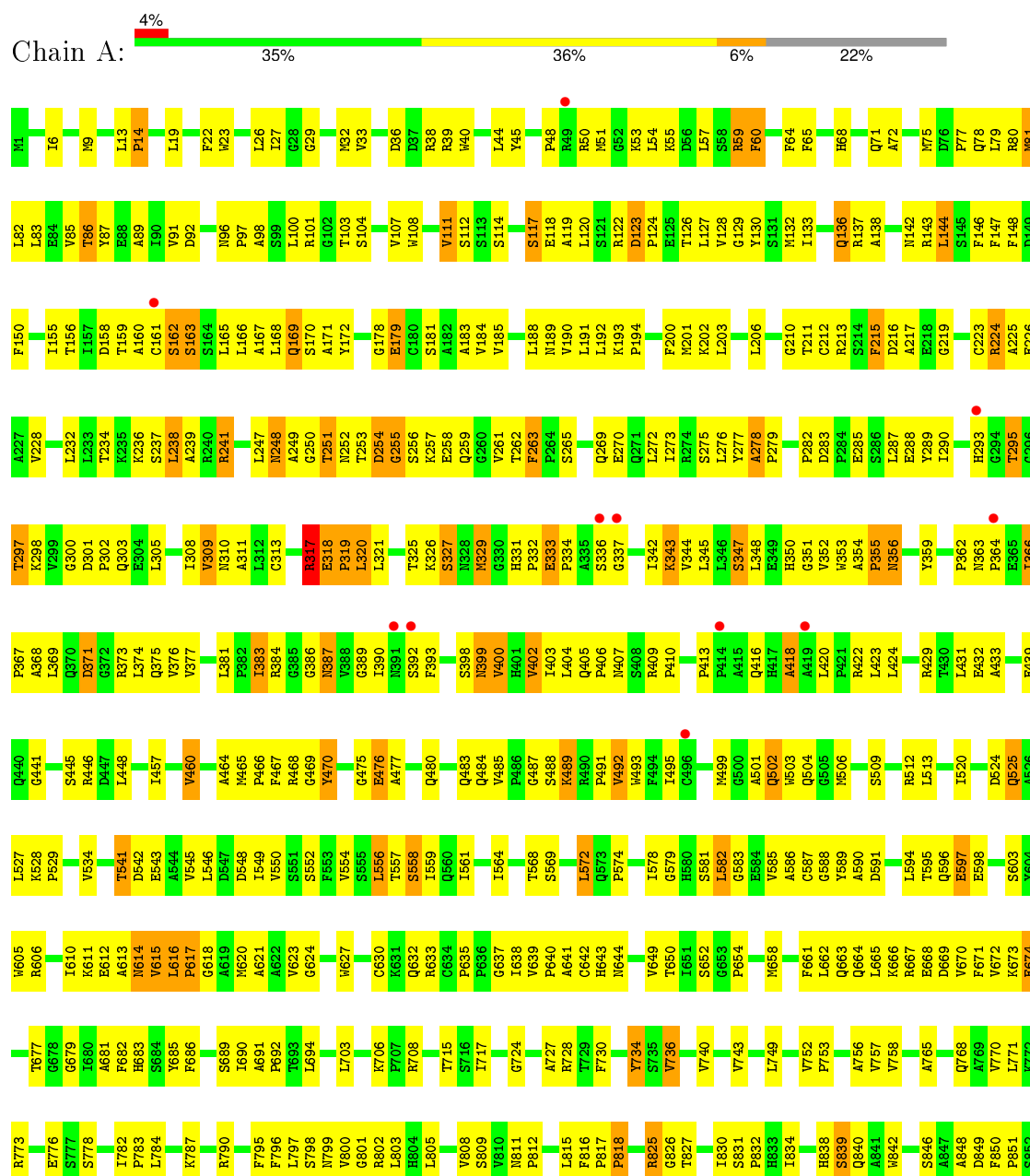
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	834	ILE	UNK	CONFLICT SEE REMARK 9	UNP A5YV76
B	834	ILE	UNK	CONFLICT SEE REMARK 9	UNP A5YV76

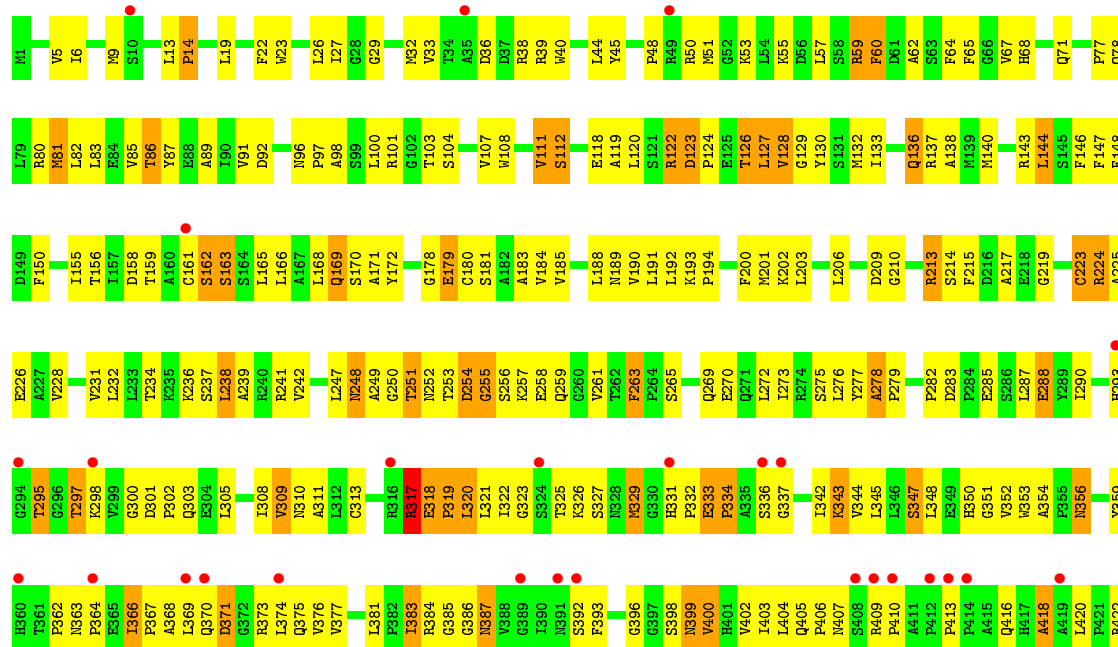
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: FATTY ACID SYNTHASE



V1853	L1769	L1689	V1617	S1542	L1477	L1416	GLY	L1292	A1223	VAL	G1098	Q1023	S941	G853
L1864	G1770	L1689	P1618	S1543	L1477	S1417	HIS	H1293	P1224	VAL	S1101	Q1023	S941	S884
Q1855	D1773	C1693	A1619	L1544	T1480	V1418	PRO	V1294	L1225	PRO	S1102	N1024	F944	S855
R1857	L1774	C1693	E1620	R1545	S1481	E1419	LEU	G1295	L1226	GLY	S1102	N1025	E945	C856
E1858	L1774	V1695	G1621	S1549	P1483	D1420	GLY	Q1296	K1227	LEU	V1103	D1026	V946	S857
E1859	N1777	V1695	L1622	S1549	A1483	T1421	GLY	G1297	A1228	ASP	A1104	S1030	S947	S858
Q1860	H1778	V1696	A1623	H1552	P1484	S1422	MET	Q1298	G1229	GLY	P1105	S1030	D848	V861
Q1861	H1778	T1697	A1623	H1552	F1423	F1423	VAL	N1299	V1230	ALA	A1106	F1031	S949	V862
L1862	L1780	S1625	S1625	Y1553	R1424	R1424	GLY	D1300	D1231	GLN	R1107	L1032	Y862	Y862
P1863	G1781	A1554	P1626	A1554	P1488	P1488	PHE	P1301	T1232	ALA	P1108	A1034	I954	K863
A1864	G1782	L1556	L1628	P1556	S1489	V1426	LEU	A1302	A1233	PRO	Q1109	A1034	I953	K863
P1865	G1783	A1557	L1629	A1557	S1490	D1427	THR	N1303	L1234	ARG	E1110	M1035	V866	V866
	V1784	S1558	Q1630	S1558	S1491	L1429	PRO	A1305	E1235	GLY	H1111	L1036	V869	V866
P1869	F1785	C1589		C1589	L1492	K1430	GLY	P1306	M1237	PRO	K1113	M1038	W962	S870
P1870	L1786	Q1560		Q1560	L1493	D1431	GLN	GLY	A1238	GLN	P1114	S1039	E963	P871
L1871	K1787	L1493		L1493	L1432	I1432	GLY	SER	S1239	GLN	L1115	I1040	S964	Y874
L1873	V1789	L1497		L1497	L1433	L1433	GLY	LEU	P1240	SER	L1116	I1040	P965	L875
T1874	F1720	L1563	V1636	L1563	A1434	A1434	ARG	GLY	K1241	LEU	K1117	P1043	D866	V876
	A1721	C1564	P1637	C1564	D1435	D1435	HIS	LYS	M1242	PRO	F1119	Y1049	P967	H877
S1877	N1722	S1638	S1638	Y1567	D1500	D1500	LEU	A1312	K1243	ARG	T1122	L1050	F970	R883
T1879	S1723	T1639	W1640	Y1568	L1501	L1501	LEU	D1313	L1245	LEU	P1123	P1051	P970	Y874
T1879	R1724	T1569	W1640	T1569	M1503	S1438	SER	L1314	V1245	LEU	H1124	R1052	T972	R883
L1795	T1726	S1570	E1644	S1570	N1504	R1439	GLN	L1315		ALA	F1125	R1053	T972	P887
L1796	S1727	L1571	E1644	S1571	V1505	P1440	GLN	L1316	L1248	ALA	E1126	F1054	T972	P887
	S1727	H1572	S1647	H1572	Y1506	V1441	THR	G1337	A1249	ALA	C1129	R1057	A975	G888
P1882	E1729	F1573	P1648	F1573	R1507	W1442	LEU	N1318	G1250	CYS	T1122	P1055	V976	G888
P1883	E1729	R1574	P1649	R1574	D1508	M1444	GLY	A1320	G1251	ASN	P1123	S1056	D977	T889
K1885	V1732	D1575	T1650	D1575	G1509	M1444	GLY	L1319	Q1252	LEU	H1124	R1057	P978	G890
S1886	L1733	V1576	V1651	V1576	A1510	V1446	ALA	A1320	Q1253	GLN	F1125	R1057	P978	L894
Y1887	R1734	V1652	Y1652	V1652	V1511	V1446	THR	ALA	Y1255	ASN	E1126	R1057	P978	T895
V1888	H1735	T1653	T1653	T1580	A1512	G1447	LEU	THR	S1256	GLY	T1134	H1064	D980	W896
	T1736	G1581	G1581	G1581	A1513	C1448	LEU	GLY	R1257	ASN	A1135	R1065	S981	T895
T1889	K1739	K1582	K1582	K1582	F1514	S1449	ASP	GLY	R1258	LEU	LEU	K1066	T982	W896
L1893	G1740	S1584	S1584	S1584	H1516	S1451	PRO	PRO	P1259	LEU	GLN	Q1067	T982	L899
G1894	D1742	P1585	P1585	P1585	F1517	G1452	ALA	ALA	L1261	GLU	GLU	Y1069	F985	A902
G1895	L1743	W1592	W1592	W1592	V1517	G1452	VAL	VAL	L1262	LEU	LEU	T1070	S888	L903
F1896	L1743	L1593	L1593	L1593	V1457	V1457	VAL	VAL	L1267	GLY	D1073	T1074	Q989	S904
	N1746	E1596	E1596	E1596	M1456	M1456	ASN	GLY	V1267	VAL	GLN	T1074	Y993	Q905
Q1899	S1747	R1595	R1595	R1595	V1457	V1457	ASN	ASN	D1269	LEU	CYS	A1077	D995	L907
W1903	L1748	C1597	C1597	C1597	L1460	L1460	MET	MET		LEU	ARG	GLY	D995	V913
K1911	Q1754	E1602	E1602	E1602	R1461	R1461	ALA	ALA	Y1272	GLN	GLY	V1082	L998	F914
L1912	Q1754	F1603	F1603	F1603	K1462	K1462	THR	THR	T1273	GLU	ALA	D1083	E915	F914
V1913	L1753	L1599	L1599	L1599	F1402	F1402	LEU	LEU	A1274	ARG	GLN	R1084	D916	E915
L1914	I1673				L1403	L1403	LYS	LYS	T1275	PRO	ALA	N1085	Y1001	V917
T1915	H1674	E1602	E1602	E1602	G1464	G1464	GLY	GLY	D1276	LEU	LEU	L1086	D1002	D916
S1916	S1675	A1531	A1531	A1531	G1466	G1466	GLY	G1341	R1277	LEU	GLN	N1087	Y1003	L925
R1917	G1676	F1532	F1532	F1532	Q1406	Q1406	GLY	G1342	H1278	LEU	THR	T1088	F1006	T930
L1917	S1677	V1533	V1533	V1533	Q1407	Q1407	ASP	F1343	P1279	ASP	LYS	V1089	F1007	V931
G1921	G1678	N1534	N1534	N1534	T1408	T1408	ALA	L1344	A1285	PRO	VAL	N1090	Q1008	V931
T1922	Q1762	G1610	G1610	G1610	P1409	P1409	LEU	L1345	Q1286	PRO	ALA	A1091	L1009	E934
	H1763	R1611	R1611	R1611	C1471	C1471	LYS	L1346	G1286	ALA	GLN	L1092	V1010	V935
	G1764	L1536	L1536	L1536	D1411	D1411	GLY	H1347	A1287	GLY	GLN	G1093	L1011	R936
	R1765	S1537	S1537	S1537	G1411	G1411	THR	T1346	K1288	GLY	GLY	A1094	D1014	L937
	F1766	R1538	R1538	R1538	S1412	S1412	LEU	T1349	L1289	LYS	LYS	L1095	D1015	L938
Q1925	H1848	G1614	G1614	G1614	V1413	V1413	LEU	L1349	E1290	LYS	GLY	F1096	L1016	E939
A1926	L1767	G1615	G1615	G1615	V1414	V1414	LEU	L1349	L1220	LYS	GLY	F1096	D1016	E939
Q1928	V1852	M1616	M1616	M1616	L1541	L1541	ALA	ALA	Q1291	D1222	MET	L1097		A940





SER	VAL	ARG	GLY	ALA	LEU	ALA	PRO	GLU	SER	GLY	G1998	R1921	A1844	H1763	L1687	M1614	G1539
ARG	VAL	ALA	GLY	THR	ILE	THR	THR	ASP	THR	THR	M2001	T1922	H1348	G1764	A1688	G1615	D1940
GLY	ARG	THR	GLY	GLY	PRO	GLY	GLY	PRO	LEU	LEU	L2002	Q1925		F1766	L1689	M1616	S1542
GLY	GLY	ASN	LEU	ASN	ASN	VAL	VAL	VAL	ASP	VAL	D2003	A1926	K1851	L1767	R1694	P1613	S1543
ALA	THR	SER	CYS	GLN	GLN	ARG	GLY	ARG	LEU	LEU	R2005	R1927	V1852	R1693	R1695	I1544	I1545
TYR	LEU	PHE	THR	THR	THR	GLN	ASP	GLN	LEU	LEU	T2006	R1930	V1853	I1769	F1696	L1622	
GLY	ALA	ARG	ALA	ALA	ALA	THR	ASP	ALA	ASP	ASP	R1931	R1930	I1854	G1770	T1697	S1625	C1548
ASP	VAL	PHE	PHE	PHE	VAL	VAL	SER	THR	SER	SER	W1856	W1932	V1856	D1773	T1698	V1626	P1550
LEU	ALA	ASP	ALA	ALA	ALA	LEU	LEU	LEU	LEU	LEU	R1933	R1934	V1857	L1774		L1627	S1549
GLY	GLY	GLY	PRO	GLY	GLY	ASN	MET	ASN	MET	GLY	C2010		E1858	E1703		C1628	L1551
ALA	THR	ALA	GLY	GLY	THR	LEU	GLY	LEU	GLY	GLY	L2013	V1937	E1859	K1704		L1629	H1552
ASP	VAL	HIS	SER	SER	THR	SER	VAL	SER	VAL	VAL	D2014	Q1938	E1860	H1705		Q1630	Y1553
TYR	ASP	HIS	THR	THR	THR	THR	GLU	THR	GLU	GLU	Y2015	V1939	Q1861	A1706		H1631	A1554
ASN	ASN	PHE	GLN	GLN	LEU	LEU	VAL	GLN	VAL	VAL	F2016	L1940	G1862	Y1707		L1555	L1555
LEU	LEU	VAL	VAL	VAL	ILE	VAL	ARG	VAL	ARG	ARG	V2017	L1941	P1863	G1781		V1636	P1556
SER	SER	THR	LEU	ASN	THR	ASN	ILE	ASN	ILE	ILE	I2018		A1864	M1782		R1711	A1557
GLN	GLN	ALA	ALA	PRO	ALA	PRO	LEU	PRO	LEU	LEU	F2019	S1944	P1865	A1783		T1639	S1558
VAL	VAL	THR	SER	GLY	THR	GLY	LEU	GLY	LEU	LEU	S2020		L1868	F1712		W1640	C1559
CYS	CYS	HIS	TYR	TYR	TYR	GLY	ARG	GLY	ARG	ARG	S2021	G1951	P1869	F1720		T1641	Q1560
ASP	ASP	ALA	TYR	TYR	TYR	PRO	GLU	PRO	GLU	GLU	V2022	A1952	P1870	A1721		L1642	L1563
GLY	GLY	GLN	ILE	ILE	ILE	THR	HIS	THR	HIS	THR	S2023	R1953	L1871	N1722		E1643	C1564
LYS	LYS	VAL	VAL	VAL	VAL	LEU	ASP	LEU	ASP	LEU	C2024	S1954	A1872	N1723		S1565	S1565
VAL	VAL	ARG	CYS	THR	THR	THR	THR	THR	THR	THR	R2026	L1955	L1873	A1724		V1566	Y1567
SER	SER	ALA	ILE	ILE	ARG	ARG	VAL	ARG	VAL	VAL	G2027	T1956	T1874	D1725		P1649	Y1568
HIS	HIS	MET	GLN	GLN	LEU	ASN	LEU	ASN	LEU	LEU	M2028	T1957	G1875	T1726		I1650	T1569
ILE	ILE	THR	VAL	VAL	THR	SER	MET	VAL	THR	THR	Q2031	E1958	L1876	F1728		V1651	S1570
GLY	GLY	PRO	GLN	GLN	GLY	VAL	ARG	GLN	ARG	GLY	A2032	G1966	K1878	E1729		Y1652	
ASP	ASP	GLY	GLY	GLY	GLY	VAL	GLY	VAL	GLY	GLY	Y2034	G1967	T1879			T1653	F1573
HIS	HIS	ALA	ALA	ALA	ALA	ALA	ASP	ALA	ASP	ASP	F2036	L1971	P1882	V1732		Y1856	V1576
ARG	ARG	GLY	PRO	GLY	GLY	GLY	GLN	GLY	GLN	GLY	G2039	M1973	K1885	R1734		S1657	T1580
THR	THR	ALA	ARG	ARG	ARG	PRO	SER	PRO	SER	SER	A2040	V1974	S1886	H1735		G1658	G1581
LEU	LEU	GLY	ILE	ILE	ILE	LEU	LEU	LEU	LEU	LEU	E2041	L1975	Y1887	T1736		L1659	K1582
ALA	ALA	ALA	ALA	ALA	ALA	PHE	ARG	PHE	ARG	ARG	R2042	R1976	V1888			V1860	
LYS	LYS	TYR	TYR	TYR	LYS	VAL	LYS	VAL	LYS	LYS	A2043	D1977	I1889	K1739		R1661	L1583
SER	SER	MET	SER	SER	GLN	HIS	GLN	HIS	GLN	GLN	I2044	A1978	T1890	D1741		R1662	S1584
ALA	ALA	TYR	TYR	TYR	PRO	PRO	GLY	PRO	GLY	GLY	R2048	V1979	L1893	L1743		D1586	
GLY	GLY	PHE	GLY	GLY	ILE	ILE	LEU	ILE	LEU	LEU	E1981	L1980	G1894			Q1566	
GLY	GLY	PHE	ALA	ALA	GLY	GLY	SER	GLY	SER	SER	R2049	R1982	G1895	L1744		E1669	
ASN	ASN	VAL	CYS	CYS	VAL	VAL	ASP	GLY	ASP	ASP	L2056	Q1983		L1745		S1670	L1593
ILE	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR		T1984	L1898			V1671	T1594
THR	THR	PHE	ALA	ALA	ALA	ALA	THR	ALA	THR	THR		P1985	Q1999	S1747		L1672	R1595
ILE	ILE	THR	GLY	GLY	VAL	VAL	THR	VAL	THR	THR	W2060	E1986		A1749		D1596	D1597
ALA	ALA	ASP	MET	MET	PHE	PHE	ASP	PHE	ASP	ASP		F1987	W1903			S1675	M1598
THR	THR	THR	CYS	CYS	THR	THR	ALA	THR	ALA	ALA	G2064	F1988	L1904	L1753		G1676	
THR	THR	GLY	ASP	ASP	GLY	GLY	ALA	GLY	ALA	ALA	D2065	Q1989		Q1754		S1677	E1602
CYS	CYS	GLN	ASP	ASP	GLY	GLY	ASP	GLY	ASP	ASP	V2066	D1990	K1911	A1755		G1678	F1603
LEU	LEU	GLN	LEU	LEU	VAL	VAL	PRO	VAL	PRO	PRO	G2067	V1991	L1912	S1756		G1679	
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	S1992	V1913	V1913	V1757		V1680	R1506
LYS	LYS	LYS	THR	THR	THR	THR	THR	ALA	THR	THR	V2069	F1914	F1914	R1758		G1681	D1607
VAL	VAL	VAL	PRO	PRO	LYS	LYS	PRO	LYS	PRO	PRO	L2070	K1993	T1915	C1759		Q1682	
PRO	PRO	LEU	THR	THR	LEU	LEU	THR	LEU	THR	THR	E2071	P1994	T1916	A1760			
ARG	ARG	GLY	THR	THR	GLN	GLN	SER	THR	SER	SER	THR	Y1995	R1917	A1761		T1685	R1611
VAL	VAL	ALA	ASP	ASP	ILE	ILE	HIS	ILE	HIS	HIS	MET	S1997		Q1762		A1686	V1613



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.32Å 244.70Å 135.25Å 90.00° 101.65° 90.00°	Depositor
Resolution (Å)	29.50 – 3.22 29.50 – 3.22	Depositor EDS
% Data completeness (in resolution range)	94.8 (29.50-3.22) 97.6 (29.50-3.22)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.217 , 0.259 0.202 , 0.244	Depositor DCC
$R_{free}$ test set	4841 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	95.2	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 73.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 96482 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	30281	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.45	1/15302 (0.0%)	0.63	0/20792
1	B	0.41	0/15634	0.60	1/21243 (0.0%)
All	All	0.43	1/30936 (0.0%)	0.61	1/42035 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1759	CYS	CB-SG	-5.79	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1694	ARG	NE-CZ-NH1	6.90	123.75	120.30

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	14977	0	14938	1049	0
1	B	15304	0	15266	1083	0
All	All	30281	0	30204	2085	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 34.

The worst 5 of 2085 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:1694:ARG:HH11	1:B:1694:ARG:HG3	1.17	1.10
1:B:1303:ASN:H	1:B:1304:PRO:HD3	1.25	1.02
1:A:1473:LEU:HD21	1:A:1503:MET:HG2	1.36	1.02
1:A:165:LEU:HD23	1:A:400:VAL:HG22	1.37	1.02
1:B:1456:MET:HG2	1:B:2036:PHE:HB2	1.41	1.01

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	1948/2512 (78%)	1586 (81%)	282 (14%)	80 (4%)	3	27
1	B	1992/2512 (79%)	1622 (81%)	296 (15%)	74 (4%)	4	29
All	All	3940/5024 (78%)	3208 (81%)	578 (15%)	154 (4%)	4	28

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	GLU
1	A	255	GLY
1	A	278	ALA
1	A	333	GLU
1	A	413	PRO

### 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	1624/2072 (78%)	1450 (89%)	174 (11%)	8	34
1	B	1660/2072 (80%)	1473 (89%)	187 (11%)	7	32
All	All	3284/4144 (79%)	2923 (89%)	361 (11%)	8	33

5 of 361 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1996	TYR
1	B	318	GLU
1	B	1823	VAL
1	A	2028	ASN
1	B	127	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2086	GLN
1	B	350	HIS
1	B	1777	ASN
1	A	2103	HIS
1	B	136	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1962/2512 (78%)	-0.10	91 (4%)	36	24	63, 118, 226, 276	0
1	B	2004/2512 (79%)	0.12	141 (7%)	19	12	54, 158, 230, 276	0
All	All	3966/5024 (78%)	0.01	232 (5%)	26	16	54, 136, 229, 276	0

The worst 5 of 232 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	581	SER	8.1
1	B	496	CYS	7.6
1	B	579	GLY	7.6
1	A	1297	GLY	7.5
1	B	498	GLY	7.3

### 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 carbohydrates 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.