



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 2VZ8 / pdb_00002vz8
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.

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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

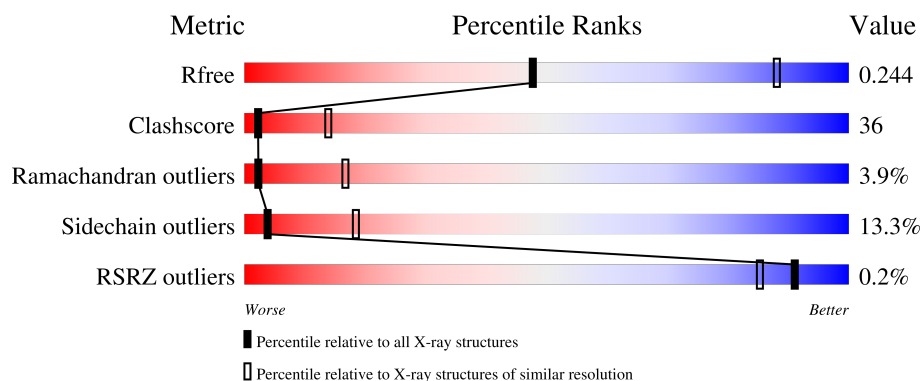
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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	2512	
1	B	2512	

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			

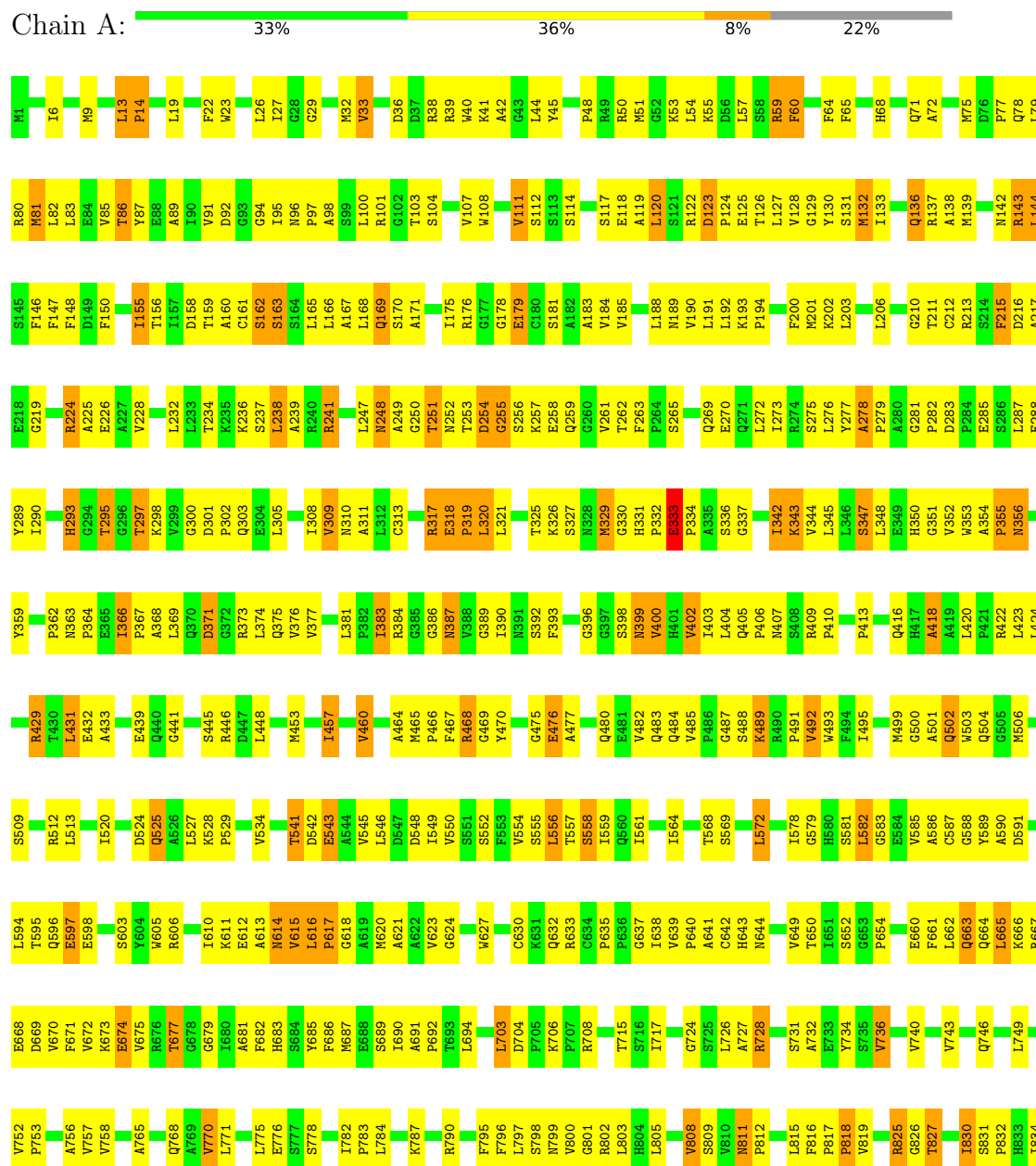
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	834	ILE	UNK	conflict	UNP A5YV76
B	834	ILE	UNK	conflict	UNP A5YV76

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.

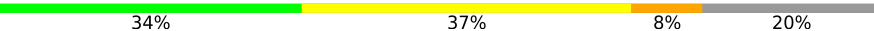
• Molecule 1: FATTY ACID SYNTHASE



L1826	V1757	G1676	S1609	V1535	R1470	L1403	MET	L1270	GLU	V1082	Y1001	V913	H383
V1830	R1758	S1677	G1610	L1536	C1471	C1404	ALA	D1271	ARG	D1083	D1002	F914	S839
F1831	G1759	G1678	R1611	S1537	L1472	Q1405	ALA	T1272	PRO	N1084	Y1003	E915	Q840
P1832	G1760	G1679	R1612	R1538	L1473	Q1406	THR	T1273	LEU	N1085	G1004	D916	
L1833	L1761	G1680	V1613	G1539	L1474	Q1407	LEU	A1274	LEU	L1086	P1005	V917	A841
L1834	Q1762	G1681	M1614	D1540	S1475	T1408	LYS	T1275	CYS	N1087	F1006	L825	W842
K1835	H1763	G1682	G1615	L1541	N1476	P1409	GLU	D1276	ASP	T1088	F1007	D843	D843
V1836	G1764	G1683	M1616	S1542	L1477	Q1410	GLU	R1277	ASP	V1089	Q1008	V844	V844
L1837	G1765	A1688	V1617	S1543	T1480	S1412	G1342	N1278	PRO	V1090	L1009	T930	S846
A1838	F1766	L1689	A1618	L1544	S1481	S1413	F1344	P1279	L1216	A1091	V931	V931	
A1839	S1690	G1691	E1620	R1545	P1482	V1414	L1346	E1283	L1217	G1092	L1011	A847	A847
L1840	L1767	G1692	G1621	S1549	A1483	F1415	L1345	A1284	GLY	G1093	D1014	E934	A848
V1841	E1768	G1693	A1622	L1564	P1484	L1416	H1347	A1285	LEU	A1094	L1015	V935	D849
L1842	L1769	H1552	L1622	E1565	E1485	L1417	H1348		LYS	L1095	L1016	V936	F850
M1843	G1770	C1693	A1623	V1567	L1486	S1417	T1349	L1289	MET	F1096	E1016	L937	P851
L1844	D1773	R1694	T1624	L1553	E1487	V1418	L1348	E1290	VAL	L1097	Q1032	L938	S852
H1848	L1774	V1695	S1625	A1554	P1488	E1419	LEU	Q1291	VAL	G1098	Q1023	E939	G853
		F1696	L1626	L1555	H1488	D1420	ALA	L1292	PRO		W1024	A940	S854
		T1697	L1627	S1489	S1489	T1421	GLY	L1293	GLY	S1101	N1025	S941	S855
		L1698	L1628	A1557	S1490	S1422	HIS	H1293	LEU	S1102	D1026	C856	C856
		V1699	L1629	S1558	S1491	F1423	PRO	V1294	ASP	V1103		F944	S857
		Q1630	Q1630	E1492	L1493	R1424	LEU	Q1296	GLY	R1106	S1030	E945	S858
				Q1560		W1425	GLY	G1297	ALA	R1107	F1031	V946	
						S1428	MET	Q1298	ALA	P1108	L1032	S947	V861
						L1429	VAL	W1299	PRO	L1033	D1033	D948	W862
						L1432	GLY	P1301	ARG	E1110	A1034	S949	K863
						L1433	PHE	A1302	GLU	H1113	M1035	N950	V866
						L1439	THR	N1303	ALA	L1112	H1037	L953	S867
						P1440	SER	A1304	PRO	K1113	M1038	I954	
						V1441	PRO	A1305	GLN	P1114	S1039	S870	S870
						W1442	GLU	A1306	GLN	L1115	I1040	P871	P871
						L1443	GLN	GLY	SER	E1117	P1043	W962	Y874
						M1444	GLY	LEU	PRO	K1118	L1048	E963	L875
						A1445	ARG	GLY	ARG	K1243	Y1049	S964	V876
						V1446	HIS	LYS	LEU	V1244	L1050	P965	D877
						G1447	LEU		LEU	V1245	L1051	D866	H878
						C1448	LEU	A1312	ALA	T1222	P1051	P967	
						S1449	SER	D1313	ALA	H1124	T1052		R883
						T1450	GLN	L1314	ALA	H124	F1053	F970	F886
						S1451		L1315	CYS	E1126	F1054	D971	P887
						G1452	D1376	V1316	GLN	T1251	T1055	T972	P887
						V1453	Q1377	C1317	LEU	C1129	S1056	V976	G888
						V1454	W1378	M1318	GLN	L1130	T1057	D977	T889
						M1455		C1319	LEU	Q1253	R1058	G890	G890
						V1457	L1387	A1320	ASN	N1133	H1064	P978	
						L1460	H1388	ALA	GLY	T1134	R1065	E964	L894
						R1461	THR	LEU	ASN	A1135	Q1066	F985	T895
						K1462	LEU	P1259	LEU	LEU	K1067		W896
						E1463	GLY	A1260	GLN	GLN	L1068	L899	
						P1464	PRO	L1261	LEU	GLU	L1069	S988	A902
						G1465	ALA	L1262	LEU	LEU	T1070	Q989	
						G1466	VAL	T1264	GLN	LEU	D1073	Y953	L903
						H1467	ALA		GLY	LEU	T1074	K994	S904
						L1468	S1399	ALA	VAL	CYS	D1073	D995	Q905
						L1469	V1400	VAL	ALA	ARG	T1074	L998	A906
							V1401	GLY	ALA	GLY	A1077		L907
							F1402	ASN	GLN	LEU			

LEU	SER	ILE	ILE	HIS	SER	GLN	PHE	THR	GLN	ALA	ILE	THR	THR	SER	THR	ILE	THR	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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● Molecule 1: FATTY ACID SYNTHASE

Chain B:  34% 37% 8% 20%

W1	L79	F147	G219	E285	V352	W5	R80	F148	G220	S286	W353	M9	V85	T156	I155	F150	L82	L83	L84	T86	H87	E88	T159	A160	G161	S162	S163	S164	G94	L165	L166	A167	L168	Q169	S170	A171	I176	R176	G177	R38	R39	W40	L44	Y45	P48	R49	R50	M51	G52	K53	L54	D56	L57	S58	R59	F60	D61	A62	S63	F64	F65	G66	Q71	W75	G76	P77	F78	Q78
L79	R80	F148	G221	S287	W354	V5	M81	F149	G222	S288	W355	M9	V86	T157	I156	F151	L83	L84	T87	H88	E89	T160	A161	G162	S164	G95	L166	L167	A168	Q170	S171	A172	I177	R177	G178	R39	R40	W41	L45	Y46	P49	R50	M52	G53	K54	L55	D57	L58	S59	R60	F61	A63	S64	F65	G67	Q72	W76	G77	P78	F79	Q79							
F147	G220	S286	W353	M9	V85	T156	I155	F150	L82	L83	L84	T86	H87	E88	T159	A160	G161	S162	S163	S164	G94	L165	L166	A167	L168	Q169	S170	A171	I176	R176	G177	R38	R39	W40	L44	Y45	P48	R49	R50	M51	G52	K53	L54	D56	L57	S58	R59	F60	D61	A62	S63	F64	F65	G66	Q71	W75	G76	P77	F78	Q78								
G219	E285	V352	W5	R80	F148	G220	S286	W353	M9	V85	T156	I155	F150	L82	L83	L84	T86	H87	E88	T159	A160	G161	S162	S163	S164	G94	L165	L166	A167	L168	Q169	S170	A171	I176	R176	G177	R38	R39	W40	L44	Y45	P48	R49	R50	M51	G52	K53	L54	D56	L57	S58	R59	F60	D61	A62	S63	F64	F65	G66	Q71	W75	G76	P77	F78	Q78			
E285	V352	W5	R80	F148	G220	S286	W353	M9	V85	T156	I155	F150	L82	L83	L84	T86	H87	E88	T159	A160	G161	S162	S163	S164	G94	L165	L166	A167	L168	Q169	S170	A171	I176	R176	G177	R38	R39	W40	L44	Y45	P48	R49	R50	M51	G52	K53	L54	D56	L57	S58	R59	F60	D61	A62	S63	F64	F65	G66	Q71	W75	G76	P77	F78	Q78				
V352	W353	A354	P355	N356	Y359	P362	N363	P364	E365	T366	P367	A368	L374	Q375	V376	V377	L381	P382	L383	R384	G385	P386	R387	S392	F393	G396	G397	S398	N399	V400	H401	V402	T403	L404	Q405	P406	N407	S408	R409	P410	P413	Q416	H417	A418	A419	L420	P421																					

S1475	P1413	F1343	L1282	G1219	V1089	D1014	E945	C856	L787	Y604	Q502	R422
N1476	V1414	L1344	E1283	L1220	V1090	L1015	V946	Y861	Q788	W605	W503	L423
L1477	F1415	L1345	A1284	D1221	A1091	E1016	S947	Y861	W770	R606	Q504	L424
	L1416	L1346	A1285	D1222	G1092		D948	Y863	Y770		G505	
T1480	S1417	H1347	K1288	A1223	G1093	Q1023	S949	H863		T610	M506	R429
T1481	T1418	L1348	L1289	A1224	A1094	Y1024	N950		L775	K611	R512	T430
P1482	E1419	L1349	L1290	A1225	L1095	H1025	L953	Y866	E776	E612	L513	L431
	D1420	LEU	Q1291	L1226	L1096	D1026	L954	S867	S777	V615	L520	E432
M1486	T1421	ALA	L1292	K1227	G1098	S1030		S870	S778	L616	I520	A433
H1487	F1422	GLY	H1293	A1228	G1098	F1031	V959		T782		Q525	E439
P1488	F1423	HIS	L1294	C1229	S1101	L1032	Y862	Y874	P783	M620	A621	Q440
	R1424	PRO	V1294	D1231	S1102	D1033	E963	Y876		A622	A526	Q441
S1491	W1425	LEU	T1295	T1232	V1103	A1034	S964	D877	L793	W623	L527	S445
		GLY	Q1296	A1233		M1036	S964	Y877	E794	G624	V534	
L1497	S1428	GLU	G1297	A1236	R1106	L1037	S964	D877	F796	L625	L448	
D1500	K1430	MET	Q1298	D1236	R1107	H1037	P967		F796	W627	W453	
L1501	D1431	VAL	W1299	E1235	P1108	M1038	P967	R883	L797	S628	V645	
V1502	I1432	PHE	P1301	N1236	Q1109	S1039		Y884	D704	W627	L546	
M1503	L1433	LEU	A1302		Q1110	I1040	F970	L885	F705	E628	I549	
M1504		THR	N1303	S1239	H1111	L1041	D971	F886	K706	C630	S552	
V1506	S1437	PRO	P1304	M1242	K1112	A1042	R973	P887	R711		S554	V460
R1507	A1436	GLN	P1306	K1243	K1113	P1043	R973	G888	W712	C634	V554	P462
	S1438	GLU	GLY	V1244	P1114	Y1049	A974	G890	T715	P635	F553	S461
G1512	R1439	GLY	LEU	V1245	I1115	L1050	V976		T716	P636	S555	V463
A1513	Y1441	GLY	LEU	E1246	K1118	P1051	D977	L894	W717	G637	L556	A464
F1514	W1442	ARG	GLY	Y1247	F1119	T1052	P978	T895	F717	I638	T557	M465
R1515	L1443	HIS	LVS	L1248	C1120	R1053	A979	N811	P639	V640	S558	P466
H1516	M1444	LEU			F1121	F1054	D980	T898	G724	P640	I559	F467
F1517	A1445	LEU	CYS	D1251	T1122	T1055	S981		P812	A641	Q560	R468
P1518	L1446	L1373	GLN	G1252	P1123	S1056	T982	A902	P817	C642	I561	G469
L1519	G1447	L1381	GLN	G1253	H1124	T1057	A983	L903	R728	H643	I564	Y470
E1520	C1448	F1382	LEU	L1254	V1125	R1058	E984	Q905	E820	N644	T568	G475
	S1449		ASN	Y1255	E1126	I1059	F985	Q905	F821	S645	A476	A477
E1525	T1450	L1387	GLY	S1256	GLY	D1060		N906	Y734	K646	S569	A478
K1526	K1526	L1388	ASN	R1257	C1129	F1061	Q988	L907	S735	D647	L570	G478
Q1527	S1451	L1389	LEU	I1258	L1130	P1062	Q989		W736	T648	L572	Q480
T1528	G1452	V1390	GLN	P1259		T1063	G990	V912	T827	T649	E481	
H1530	V1453	LEU	ALA	A1260	L1136	H1064	D991	V913	I830	V650	D575	V482
A1531	G1455	THR	GLU	L1261	Q1137		V992	F914	S831	E659	I577	V485
F1532	M1456	LEU	LEU	L1262	E1138	K1067	Y993	E915	Q746	E660	I578	F486
V1533	V1457	GLY	GLY	N1263	E1139	L1068	K994	D916	S839	F661	S581	S488
H1534	C1459	ASP	GLN	T1264		Y1069	D995	V917	Q840	L662	L582	R490
V1536	L1460	P1327	VAL		C1143	T1070	L996		I834	Q663	G583	P491
L1536	S1328	L1328	LEU	V1267	ARG	L1071	R997	L925	H838	Q664	E584	V492
S1537	V1329	V1329	ALA	M1268	GLY	Q1072	L998	T930	Q746	L665	V585	A493
R1538	A1330	A1330	GLN	D1269	LEU	D1073	L998	T931	S839	E659	A586	F494
R1539	V1331	V1331	GLU	L1270	ALA	T1074		V931	Q840	F661	C587	I495
F1402	G1332	G1332	ARG	D1271	ALA		D1002		P845	L665	G588	C496
L1403	N1333	N1333	PRO	D1272	ALA	A1077	Y1003	E934	S846		A590	G498
C1404	A1334	A1334	LEU	Y1273	LEU		G1004	V935	A847	E668	D591	M499
R1405	A1335	A1335	LEU	A1274	GLN	V1081	P1005	L937	F850		G500	A501
Q1406	A1336	A1336	CYS	T1275	THR	V1082	F1006	L937	Q746	D669		
Q1407	T1337	T1337	ASP	D1276	LVS	D1083	F1007	E939	P851	V670	G588	
T1408	L1338	L1338	ASP	R1277	VAL	R1084	Q1008	A940	S852	F671	G498	
P1409	K1339	K1339	PRO	H1276	ALA	N1085	L1009	S941	S853	V672	A590	
Q1410	E1340	E1340	PRO	P1279	GLN	L1086	V1010		G853		D591	
L1473	G1341	G1341	GLN	Q1280	GLN	L1086	L1011	F944	S854	A765	G500	
S1412	G1342	G1342	GLY	A1281	GLY	T1088			S855	V675	S603	



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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) 97.5 (29.50-3.22)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.217 , 0.259 0.205 , 0.244	Depositor DCC
R_{free} test set	4839 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	95.2	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 106.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30281	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.59	0/15302	1.00	62/20792 (0.3%)
1	B	0.54	0/15634	0.96	55/21243 (0.3%)
All	All	0.56	0/30936	0.98	117/42035 (0.3%)

There are no bond length outliers.

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1636	VAL	CA-C-N	8.25	128.76	119.93
1	A	1636	VAL	C-N-CA	8.25	128.76	119.93
1	B	1223	ALA	CA-C-N	8.08	129.94	119.84
1	B	1223	ALA	C-N-CA	8.08	129.94	119.84
1	A	500	GLY	N-CA-C	-8.02	104.78	115.21

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	14977	0	14938	1114	0
1	B	15304	0	15266	1135	0
All	All	30281	0	30204	2196	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 36.

The worst 5 of 2196 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%)	2	16
1	B	1992/2512 (79%)	1622 (81%)	296 (15%)	74 (4%)	2	17
All	All	3940/5024 (78%)	3208 (81%)	578 (15%)	154 (4%)	2	17

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%)	1412 (87%)	212 (13%)	4	19
1	B	1660/2072 (80%)	1436 (86%)	224 (14%)	4	18
All	All	3284/4144 (79%)	2848 (87%)	436 (13%)	4	18

5 of 436 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	224	ARG
1	B	821	PHE
1	B	1815	LYS
1	B	309	VAL
1	B	460	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	738	ASN
1	B	1884	HIS
1	B	1037	HIS
1	B	1530	HIS
1	A	1318	ASN

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 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	1962/2512 (78%)	-0.56	3 (0%)	91 85	63, 118, 226, 276	0
1	B	2004/2512 (79%)	-0.45	3 (0%)	92 89	54, 158, 230, 276	0
All	All	3966/5024 (78%)	-0.51	6 (0%)	91 85	54, 136, 229, 276	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1327	PRO	2.6
1	A	1312	ALA	2.4
1	B	222	TYR	2.3
1	A	1344	LEU	2.3
1	A	1451	SER	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.