



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 17, 2016 – 09:52 AM EDT

PDB ID : 5I6I
Title : Crystal structure of a dBCCP-variant of Chaetomium thermophilum acetyl-CoA carboxylase
Authors : Hunkeler, M.; Stuttfeld, E.; Hagmann, A.; Imseng, S.; Maier, T.
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027257
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) : rb-20027257

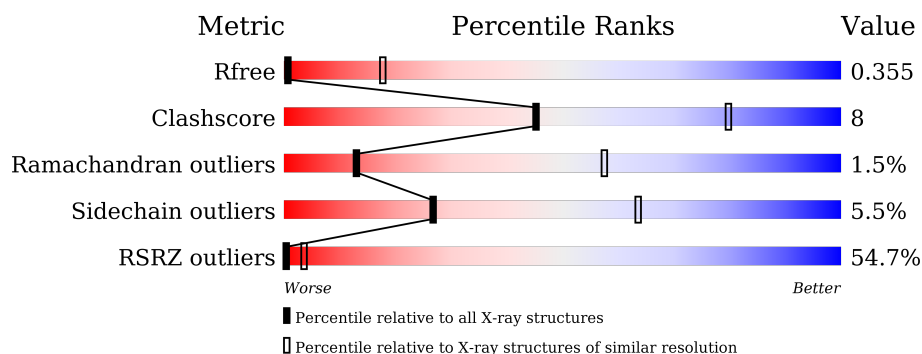
1 Overall quality at a glance

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}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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 ≥ 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	2211	<div> <div>36%</div> <div>48%</div> <div>13%</div> <div>•</div> <div>37%</div> </div>
1	B	2211	<div> <div>33%</div> <div>49%</div> <div>13%</div> <div>•</div> <div>37%</div> </div>

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.

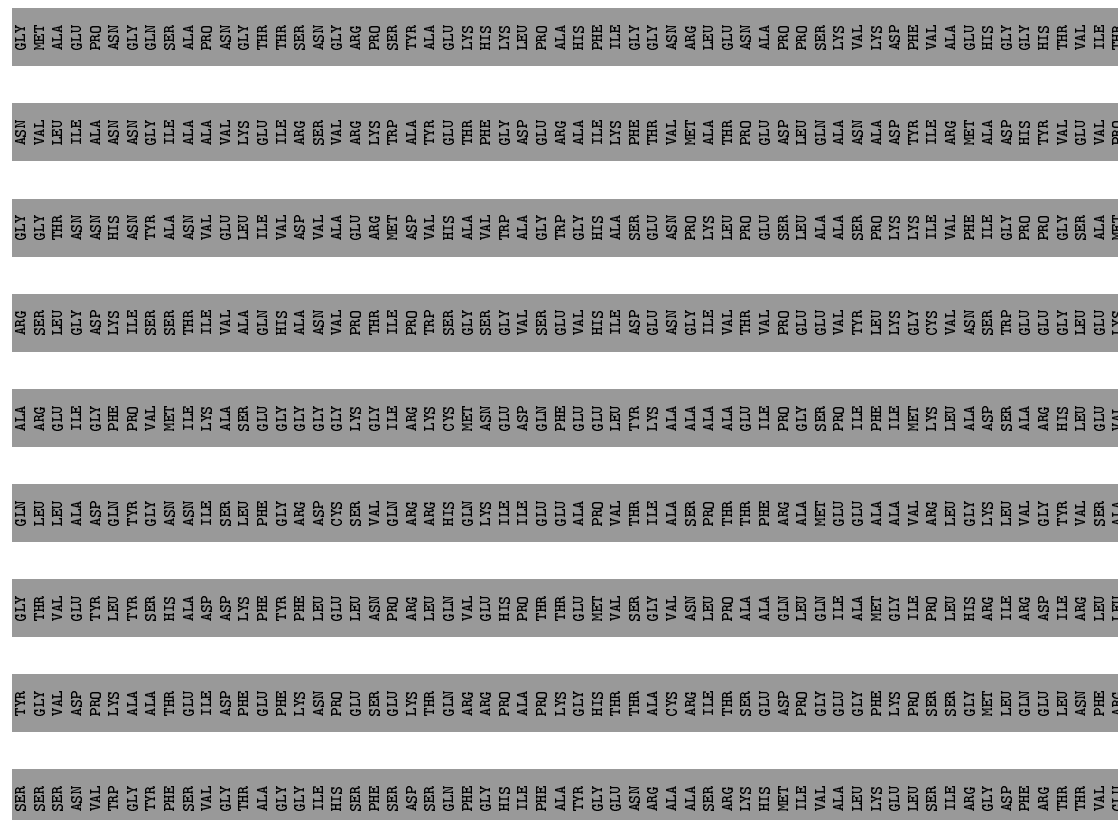
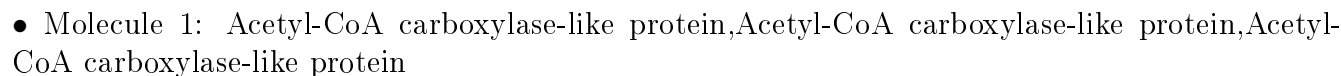
- Molecule 1 is a protein called Acetyl-CoA carboxylase-like protein,Acetyl-CoA carboxylase-like protein,Acetyl-CoA carboxylase-like protein.

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

D1705	P1619	V1521	E1431	H1351	R1289	LYS	E1162	Y1096	A1025	V965	L904	R843	LEU
E1706	E1620	S1522	V1432	I1352	V1290	GLN	R1163	Y1097	R1026	V966	E905	Q844	PRO
A1707	V1621	T1523	A1433	H1353	R1291	GLN	D1164	A1098	E1027	V967	P906	P845	GLN
K1708	P1622	P1524	V1354	V1354	R1292	PRO	F1165	L1099	L1028	T968	T908	S846	TTR
R1709	R1625	Y1525	R1451	E1355	L1293	GLY	R1166	A1100	A1100	V969	S909	A847	GLY
R1710	K1626	T1526	V1452	E1356	T1294	ILE	R1167	A1101	T1030	L970	S909	L848	S788
F1711	F1627	T1527	H1453	R1360	F1295	ALA	R1168	L1102	L1031	S971	V910	H849	P789
E1714	V1629	K1528	Q1454	I1361	L1296	ALA	H1169	E1103	CYS	R972	V910	A850	V790
V1715	V1630	R1529	A1459	G1361	C1297	ASP	S1170	V1104	ALA	R973	N912	R851	V791
T1716	A1631	G1542	N1460	E1362	R1298	LEU	Y1105	V1105	LEU	N974	L913	M852	V792
T1717	Q1543	T1543	G1461	T1364	G1299	ALA	S1172	V1106	PRO	N975	Y914	P853	V793
T1718	Q1544	Q1544	R1462	T1364	R1299	ALA	R1107	R1107	SER	N976	L915	H854	V794
E1719	D1633	Y1546	R1463	D1365	G1302	ARG	M1174	R1108	LEU	S977	D916	K855	V795
V1720	T1634	V1546	S1464	Y1368	S1303	ARG	T1175	A1109	GLU	K978	G917	L856	V796
V1721	F1635	F1549	ASP	Y1369	Y1304	ARG	Y1176	Y1110	GLU	D857	Q918	D857	V797
D1722	F1636	P1550	ASN	F1369	P1305	PRO	L1177	R1040	GLU	N979	K919	A858	Q798
D1723	K1637	F1550	ASN	T1370	S1306	GLY	A1178	Y1041	T1041	L981	R921	Q859	R799
G1724	I1638	E1551	ASP	A1372	Y1307	THR	R1179	N1114	R1044	V982	E922	L860	F900
E1725	R1657	L1552	E1469	V1373	T1308	PRO	R1180	L1115	R1044	L983	E922	T861	A801
K1726	K1658	F1553	E1470	V1374	F1310	LEU	T1181	L1116	I1047	L985	L923	Q862	V802
R1727	R1658	T1557	D1471	R1375	R1311	LEU	D1182	E1117	L1048	L986	L924	V863	L803
H1728	P1662	Q1558	T1472	P1376	G1312	GLY	E1184	Y1120	R1049	D987	I926	L864	V804
K1729	R1663	R1558	P1473	G1377	P1313	ILE	P1185	R1125	Y1052	E988	A927	R866	T806
I1730	T1664	N1559	P1474	R1378	D1314	ILE	I1186	P1156	V1053	N989	D928	A867	N807
I1731	Y1665	S1560	L1475	L1379	Y1315	GLY	R1187	F1127	Q1054	R990	L929	Q868	C808
T1732	Y1665	Y1561	R1476	ASP	A1316	GLU	K1188	Y1127	F1054	P991	L930	R869	D809
L1733	L1666	T1562	V1477	GLU	D1318	LEU	E1189	F1128	S1055	N992	L930	R870	L810
V1734	E1563	E1563	T1482	ILE	D1319	SER	V1190	I1129	R1056	K993	M932	Q871	L811
G1735	L1674	A1564	T1482	SER	S1320	THR	P1192	D1132	Y1057	P994	Y933	A872	N812
L1675	G1675	T1568	G1483	THR	I1321	V1254	P1193	F1133	G1058	N995	D935	E873	G813
L1676	L1677	I1568	G1484	A1386	I1322	V1255	P1194	ALA	E1059	V996	V936	F874	Y814
L1677	E1677	L1568	F1485	L1389	H1323	V1257	C1194	ARG	W1062	N998	E937	A876	N816
E1678	E1679	A1572	V1486	L1389	I1324	A1258	D1196	ARG	R1066	V999	Q938	Q877	Q817
V1742	M1681	K1573	I1489	E1392	E1325	R1259	L1197	LYS	P1067	K1000	Q939	Q878	V818
C1744	P1682	Q1575	L1491	L1392	P1326	D1260	L1198	SER	D1068	K1001	F940	L879	V819
L1745	H1683	P1576	L1492	D1261	S1327	D1261	D1199	GLY	D1068	H1002	S941	L880	M820
E1684	F1684	E1493	A1403	A1262	L1328	A1262	ALA	ASN	R1069	L1003	G942	R881	Q821
N1685	N1685	E1405	L1404	E1263	G1329	G1264	GLN	GLN	E1070	H1004	R943	V882	Q822
V1686	V1686	I1406	E1406	G1265	F1330	G1265	L1204	THR	V1071	P1005	R944	F883	K823
A1687	A1687	I1582	K1495	N1266	E1333	N1266	L1204	THR	E1074	V1006	L945	N884	L824
H1688	H1688	V1588	E1501	D1267	L1334	D1267	GLU	SER	V1075	L1007	Q946	K885	K825
N1689	N1689	Y1588	V1502	E1268	G1335	E1268	L1206	SER	V1075	R1008	D947	F886	E826
V1690	V1690	V1503	V1503	E1269	R1336	E1269	L1207	SER	V1075	R1009	E948	L887	F827
P1691	P1691	Y1504	N1410	I1270	L1337	I1270	MET	HIS	S1078	T1011	E949	D888	E828
A1692	A1692	Q1592	N1415	S1338	S1338	S1338	GLN	MET	Y1080	E1012	A950	D889	E829
K1693	K1693	N1594	H1416	H1416	T1342	LYS	L1211	VAL	T1081	E1013	N890	N890	V830
P1694	P1694	L1595	W1417	W1417	P1340	LEU	P1212	SER	V1082	E1014	L952	P892	L831
E1695	E1695	A1596	F1418	F1418	K1341	ALA	L1274	VAL	F1083	S1015	L954	H893	D832
A1696	A1696	E1597	H1423	H1423	L1342	ALA	ALA	V1153	F1083	S1016	L954	H893	D833
G1697	G1697	V1598	T1424	T1424	P1344	GLU	GLU	S1155	V1085	Q1017	D956	T895	P834
F1698	F1698	K1599	T1425	T1425	T1345	THR	THR	P1156	V1085	Q1017	D956	T895	P834
K1699	K1699	R1600	Q1426	Q1426	F1346	LYS	LYS	P1157	T1087	A1019	K953	P892	R832
R1771	R1771	Y1600	W1427	W1427	T1347	ASP	ASP	A1158	F1089	V1021	K959	D898	P837
L1701	L1701	V1630	H1517	H1517	T1347	LYS	LYS	A1158	F1089	V1021	K959	D898	P837
Y1702	Y1702	R1617	L1518	L1518	Q1349	LYS	LYS	T1159	F1090	S1022	D960	L899	V838
L1703	L1703	L1617	A1429	A1429	N1349	ASP	ASP	T1159	F1090	S1022	D960	L899	V838
S1704	S1704	T1618	D1430	D1430	K1350	R1288	ARG	V1161	A1091	K1024	K964	T903	S842



E1563	C1581	R1476	ASP	S1303	PRO	R1179	R1119	L1037	T968	L907	L847	LEU	GLY	ALA	TYR
A1564	I1582	V1477	GLU	S1306	GLY	R1180	Y1120	E1038	T969	T908	L848	PRO	LEU	GLY	LEU
A1573	I1582	I1478	ILE	T1181	THR	T1181	H1121	E1039	T970	T909	H849	GLN	LEU	GLY	ILE
K1574	D1399	S1483	SER	Y1307	PRO	D1182	D1122	R1040	S971	V910	H850	TTR	VAL	LEU	LYS
Q1575	A1403	G1484	THR	T1308	LEU	D1183	E1123	R972	R973	L911	H851	GLY	LEU	LYS	LEU
P1576	I1406	F1485	ARG	T1309	LEU	E1124	E1124	M1044	R974	L912	H852	GLY	LEU	LYS	LEU
		V1486	LEU	F1310	LEU	R1185	R1125	L1048	R975	L913	H853	VAL	GLN	GLN	GLU
			GLU		GLU	I1186	Y1126		R976	L914	H854	VAL	GLN	GLN	THR
			GLY	P1313	GLY	R1187	Y1127		R976	L915	H855	PRO	GLN	GLN	THR
			ILE	D1314	ILE	K1188	I1129	V1052	S977	D916	L856	SER	VAL	VAL	THR
			GLY	Y1315	GLY	G1189	I1129	Y1053	S978	D917	L857	SER	VAL	VAL	THR
			LEU	A1316	LEU	V1190	E1130	Q1054	R979	Q918	H858	ASN	ASP	ASP	GLU
			LEU	A1317	LEU	I1191	R1131	Q1055	R980	Q919	H859	VAL	ILE	ILE	GLU
			SER	D1318	SER	V1192	D1132	R1056	L981	A920	L860	LEU	LEU	ASN	ASN
				D1319		P1193	F1133		V982	R921	T861	TRP	TYR	TYR	THR
					A1253		ALA	E1059		E922	Q798	LYS	LYS	LYS	THR
					V1254		LEU			L923	H862	THR	THR	THR	THR
					N1255		ARG			L924	H863	GLU	GLU	GLU	THR
					N1256		LEU			L925	H864	VAL	VAL	VAL	THR
					V1257		LYS			L926	H865	ALA	ALA	ALA	GLY
					A1258		SER				H866	THR	THR	THR	TRP
					V1259		GLY				H867	ASP	ASP	ASP	LEU
					R1260		ALA				H868	THR	THR	THR	LEU
							ASN				H869	ILE	ILE	ILE	GLU
							GLN				H870	ILE	ILE	ILE	GLU
							THR				H871	THR	THR	THR	LEU
							GLU				H872	GLY	GLY	GLY	SER
							SER				H873	LEU	LEU	LEU	LYS
							SER				H874	ARG	ARG	ARG	LYS
							MET				H875	LYS	LYS	LYS	THR
							MET				H876	THR	THR	THR	ALA
							GLN				H877	LEU	LEU	LEU	ALA
							SER				H878	THR	THR	THR	GLU
							VAL				H879	VAL	VAL	VAL	ARG
							LEU				H880	GLU	GLU	GLU	PRO
							ALA				H881	GLN	GLN	GLN	ASP
							HIS				H882	GLU	GLU	GLU	THR
							LYS				H883	ASN	ASN	ASN	ASN
							LYS				H884	VAL	VAL	VAL	LEU
							GLU				H885	ASP	ASP	ASP	ALA
							LYS				H886	THR	THR	THR	ILE
							GLU				H887	TYR	TYR	TYR	ILE
							LYS				H888	ARG	ARG	ARG	ILE
							ASP				H889	GLY	GLY	GLY	CYS
							LYS				H890	ALA	ALA	ALA	ALA
							ASP				H891	ILE	ILE	ILE	VAL
							GLY				H892	ASP	ASP	ASP	ILE
							ILE				H893	PRO	PRO	PRO	ALA
							ALA				H894	SER	SER	SER	ALA
							GLY				H895	SER	SER	SER	HIS
							THR				H896	ARG	ARG	ARG	THR
							LEU				H897	VAL	VAL	VAL	GLU
							ALA				H898	GLY	GLY	GLY	SER
							ASP				H899	VAL	VAL	VAL	GLU
							LEU				H900	ALA	ALA	ALA	LYS
							LEU				H901	GLN	GLN	GLN	SER
							ALA				H902	THR	THR	THR	LEU
							GLN				H903	PHE	PHE	PHE	ALA
							ARG				H904	VAL	VAL	VAL	ASP
							ARG				H905	GLY	GLY	GLY	TYR
							ARG				H906	GLN	GLN	GLN	ARG
							ARG				H907	GLN	GLN	GLN	ARG
							ARG				H908	GLN	GLN	GLN	ARG
							ARG				H909	GLN	GLN	GLN	ARG
							ARG				H910	GLN	GLN	GLN	ARG
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							ARG				H914	GLN	GLN	GLN	ARG
							ARG				H915	GLN	GLN	GLN	ARG
							ARG				H916	GLN	GLN	GLN	ARG
							ARG				H917	GLN	GLN	GLN	ARG
							ARG				H918	GLN	GLN	GLN	ARG
							ARG				H919	GLN	GLN	GLN	ARG
							ARG				H920	GLN	GLN	GLN	ARG
							ARG				H921	GLN	GLN	GLN	ARG
							ARG				H922	GLN	GLN	GLN	ARG
							ARG				H923	GLN	GLN	GLN	ARG
							ARG				H924	GLN	GLN	GLN	ARG
							ARG				H925	GLN	GLN	GLN	ARG
							ARG				H926	GLN	GLN	GLN	ARG
							ARG				H927	GLN	GLN	GLN	ARG
							ARG				H928	GLN	GLN	GLN	ARG
							ARG				H929	GLN	GLN	GLN	ARG
							ARG				H930	GLN	GLN	GLN	ARG
							ARG				H931	GLN	GLN	GLN	ARG
							ARG				H932	GLN	GLN	GLN	ARG
							ARG				H933	GLN	GLN	GLN	ARG
							ARG				H934	GLN	GLN	GLN	ARG
							ARG				H935	GLN	GLN	GLN	ARG
							ARG				H936	GLN	GLN	GLN	ARG
							ARG				H937	GLN	GLN	GLN	ARG
							ARG				H938	GLN	GLN	GLN	ARG
							ARG				H939	GLN	GLN	GLN	ARG
							ARG				H940	GLN	GLN	GLN	ARG
							ARG				H941	GLN	GLN	GLN	ARG
							ARG				H942	GLN	GLN	GLN	ARG
							ARG				H943	GLN	GLN	GLN	ARG
							ARG				H944	GLN	GLN	GLN	ARG
							ARG				H945	GLN	GLN	GLN	ARG
							ARG				H946	GLN	GLN	GLN	ARG
							ARG				H947	GLN	GLN	GLN	ARG
							ARG				H948	GLN	GLN	GLN	ARG
							ARG				H949	GLN	GLN	GLN	ARG
							ARG				H950	GLN	GLN	GLN	ARG
							ARG				H951	GLN	GLN	GLN	ARG
							ARG				H952	GLN	GLN	GLN	ARG
							ARG				H953	GLN	GLN	GLN	ARG
							ARG				H954	GLN	GLN	GLN	ARG
							ARG				H955	GLN	GLN	GLN	ARG
							ARG				H956	GLN	GLN	GLN	ARG
							ARG				H957	GLN	GLN	GLN	ARG
							ARG				H958	GLN	GLN	GLN	ARG
							ARG				H959	GLN	GLN	GLN	ARG
							ARG				H960	GLN	GLN	GLN	ARG
							ARG				H961	GLN	GLN	GLN	ARG
							ARG				H962	GLN	GLN	GLN	ARG
							ARG				H963	GLN	GLN	GLN	ARG
							ARG				H964	GLN	GLN	GLN	ARG
							ARG				H965	GLN	GLN	GLN	ARG
							ARG				H966	GLN	GLN	GLN	ARG
							ARG				H967	GLN	GLN	GLN	ARG
							ARG				H968	GLN	GLN	GLN	ARG
							ARG				H969	GLN	GLN	GLN	ARG
							ARG				H970	GLN	GLN	GLN	ARG
							ARG				H971	GLN	GLN	GLN	ARG
							ARG				H972	GLN	GLN	GLN	ARG
							ARG				H973	GLN	GLN	GLN	ARG
							ARG				H974	GLN	GLN	GLN	ARG
							ARG				H975	GLN	GLN	GLN	ARG
							ARG				H976	GLN	GLN	GLN	ARG
							ARG				H977	GLN	GLN	GLN	ARG
							ARG				H978	GLN	GLN	GLN	ARG
							ARG				H979	GLN	GLN	GLN	ARG
							ARG				H980	GLN	GLN	GLN	ARG
							ARG				H981	GLN	GLN	GLN	ARG
							ARG				H982	GLN	GLN	GLN	ARG
							ARG				H983	GLN	GLN	GLN	ARG</



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	462.20 Å 462.20 Å 204.64 Å 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) 99.8 (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 8.33 Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.297 , 0.324 0.322 , 0.355	Depositor DCC
R_{free} test set	548 reflections (4.53%)	DCC
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 , 897.4	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	0.76	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, 0.375 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	0.41	0/11401	0.64	0/15435
1	B	0.41	0/11458	0.63	0/15511
All	All	0.41	0/22859	0.63	0/30946

There are no bond length outliers.

There are no bond angle outliers.

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	11224	0	11148	178	0
1	B	11221	0	11191	174	0
All	All	22445	0	22339	347	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 347 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	13	57
1	B	1380/2211 (62%)	1249 (90%)	110 (8%)	21 (2%)	13	57
All	All	2753/4422 (62%)	2478 (90%)	233 (8%)	42 (2%)	13	57

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	943	ARG
1	A	1156	SER
1	A	1516	MET
1	A	1784	GLN
1	A	1864	SER

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	1208/1879 (64%)	1138 (94%)	70 (6%)	25	61
1	B	1215/1879 (65%)	1151 (95%)	64 (5%)	28	64
All	All	2423/3758 (64%)	2289 (94%)	134 (6%)	27	63

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2022	PHE
1	B	883	PHE
1	B	1965	TRP
1	A	2088	LEU
1	A	2234	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1415	ASN

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 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 ⓘ

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%)	3.37	787 (56%) 0 3	25, 211, 483, 500	0
1	B	1394/2211 (63%)	3.07	734 (52%) 0 4	5, 245, 486, 500	0
All	All	2781/4422 (62%)	3.22	1521 (54%) 0 3	5, 230, 485, 500	0

The worst 5 of 1521 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	875	PRO	21.0
1	A	1155	SER	18.6
1	B	874	PHE	18.3
1	A	1685	ASN	18.2
1	A	926	ILE	17.4

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 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.