



wwPDB X-ray Structure Validation Summary Report

Jan 31, 2016 – 09:51 PM GMT

PDB ID : 1QXP
Title : Crystal Structure of a mu-like calpain
Authors : Pal, G.P.; Veyra, T.D.; Elce, J.S.; Jia, Z.
Deposited on : 2003-09-08
Resolution : 2.80 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 : 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

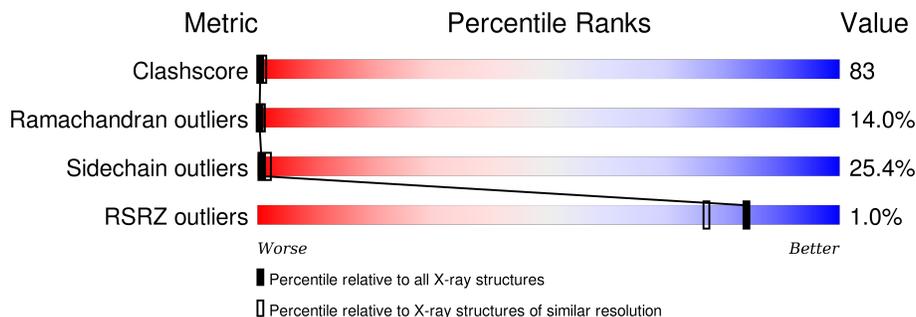
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	900	
1	B	900	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 12368 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 mu-like calpain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	783	6053	3846	1037	1143	27	0	0	0
1	B	788	6003	3830	1015	1129	29	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	SER	CYS	ENGINEERED	UNP P97571
B	105	SER	CYS	ENGINEERED	UNP P97571
A	702A	GLY	-	CLONING ARTIFACT	UNP Q07009
A	702B	LYS	-	CLONING ARTIFACT	UNP Q07009
A	702C	LEU	-	CLONING ARTIFACT	UNP Q07009
A	702D	ALA	-	CLONING ARTIFACT	UNP Q07009
A	702E	ALA	-	CLONING ARTIFACT	UNP Q07009
A	702F	ALA	-	CLONING ARTIFACT	UNP Q07009
A	702G	ILE	-	CLONING ARTIFACT	UNP Q07009
A	702H	GLU	-	CLONING ARTIFACT	UNP Q07009
A	702I	HIS	-	EXPRESSION TAG	UNP Q07009
A	702J	HIS	-	EXPRESSION TAG	UNP Q07009
A	702K	HIS	-	EXPRESSION TAG	UNP Q07009
A	702L	HIS	-	EXPRESSION TAG	UNP Q07009
A	702M	HIS	-	EXPRESSION TAG	UNP Q07009
A	702N	HIS	-	EXPRESSION TAG	UNP Q07009
B	702A	GLY	-	CLONING ARTIFACT	UNP Q07009
B	702B	LYS	-	CLONING ARTIFACT	UNP Q07009
B	702C	LEU	-	CLONING ARTIFACT	UNP Q07009
B	702D	ALA	-	CLONING ARTIFACT	UNP Q07009
B	702E	ALA	-	CLONING ARTIFACT	UNP Q07009
B	702F	ALA	-	CLONING ARTIFACT	UNP Q07009
B	702G	ILE	-	CLONING ARTIFACT	UNP Q07009
B	702H	GLU	-	CLONING ARTIFACT	UNP Q07009
B	702I	HIS	-	EXPRESSION TAG	UNP Q07009

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	702J	HIS	-	EXPRESSION TAG	UNP Q07009
B	702K	HIS	-	EXPRESSION TAG	UNP Q07009
B	702L	HIS	-	EXPRESSION TAG	UNP Q07009
B	702M	HIS	-	EXPRESSION TAG	UNP Q07009
B	702N	HIS	-	EXPRESSION TAG	UNP Q07009

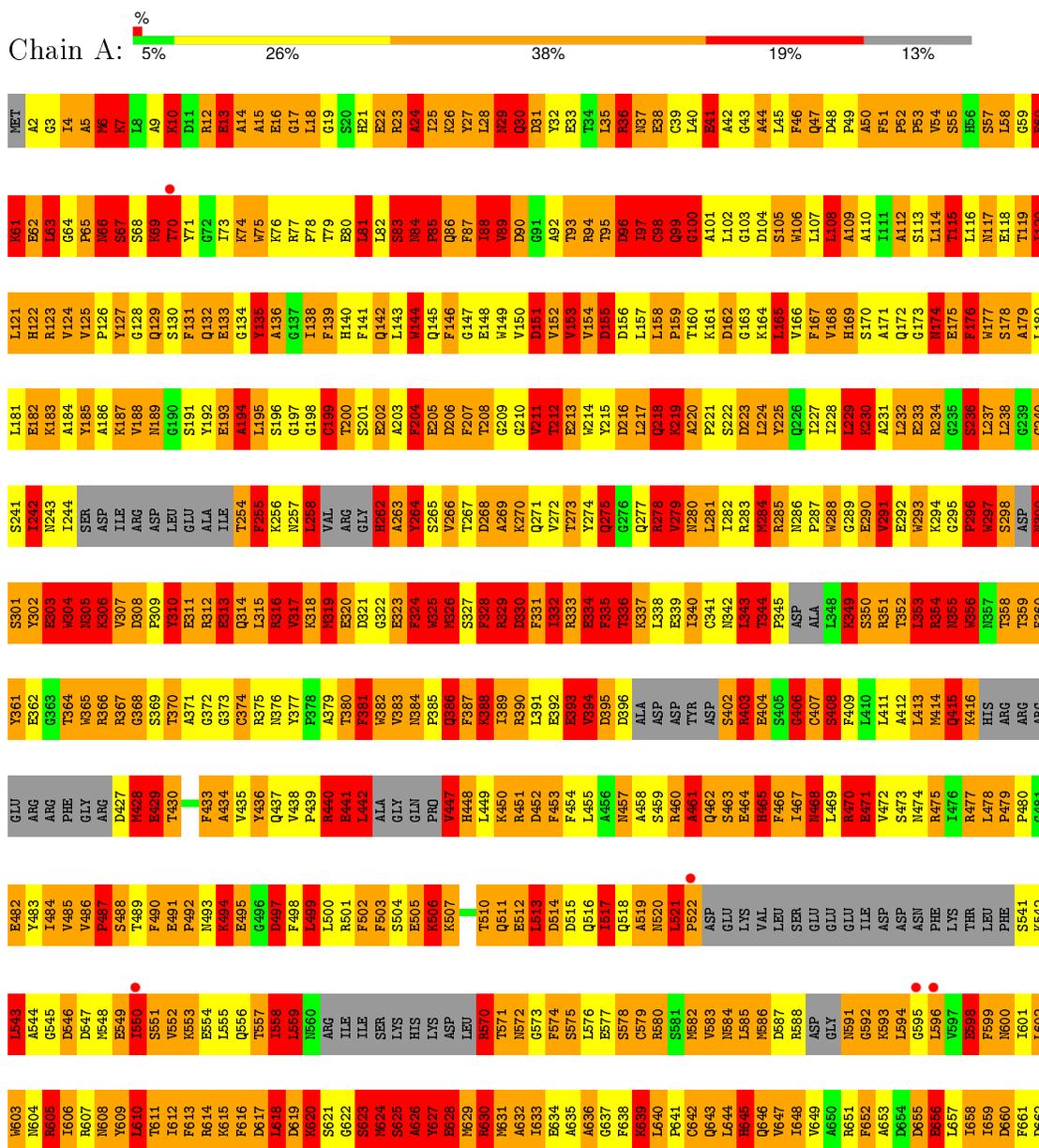
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	172	Total O 172 172	0	0
2	B	140	Total O 140 140	0	0

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 ($RSRZ > 2$). 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: mu-like calpain



1601	SER	1602	LYS	1603	LEU	1604	ALA	1605	GLY	1606	ASP	1607	ASP	1608	MET	1609	GLU	1610	L610	1611	S551	1612	V552	1613	K553	1614	K554	1615	L555	1616	F556	1617	D557	1618	L558	1619	L559	1620	L560	1621	ARG	1622	ARG	1623	F501	1624	F502	1625	S504	1626	G444	1627	G443	1628	F433	1629	F432	1630	I431	1631	A430	1632	G372	1633	G373	1634	C374	1635	R375	1636	F376	1637	V377	1638	P378	1639	A379	1640	T380	1641	F381	1642	V382	1643	V383	1644	N384	1645	P385	1646	Q386	1647	F387	1648	K388	1649	L389	1650	R390	1651	L391	1652	E392	1653	E393	1654	F394	1655	L455	1656	A456	1657	L457	1658	A458	1659	S459	1660	N520	1661	L521	1662	P522	1663	S463	1664	E464	1665	S465	1666	F466	1667	L467	1668	N468	1669	L469	1670	R470	1671	E471	1672	I472	1673	A473	1674	S474	1675	L475	1676	L476	1677	R477	1678	L478	1679	F479	1680	L480	1681	L481	1682	L482	1683	G573	1684	F574	1685	D575	1686	L576	1687	L577	1688	E578	1689	C579	1690	R580	1691	S581	1692	V582	1693	V583	1694	V584	1695	L585	1696	P586	1697	D587	1698	ARG	1699	ASP	1700	GLY	1701	GLY	1702	ASP	1703	L594	1704	D594	1705	G595	1706	D596	1707	PHE	1708	K537	1709	T538	1710	L539	1711	F540	1712	L540	1713	L541	1714	L542	1715	L543	1716	L544	1717	L545	1718	L546	1719	L547	1720	L548	1721	L549	1722	L550	1723	L551	1724	L552	1725	L553	1726	L554	1727	L555	1728	L556	1729	L557	1730	L558	1731	L559	1732	L560	1733	L561	1734	L562	1735	L563	1736	L564	1737	L565	1738	L566	1739	L567	1740	L568	1741	L569	1742	L570	1743	L571	1744	L572	1745	L573	1746	L574	1747	L575	1748	L576	1749	L577	1750	L578	1751	L579	1752	L580	1753	L581	1754	L582	1755	L583	1756	L584	1757	L585	1758	L586	1759	L587	1760	L588	1761	L589	1762	L590	1763	L591	1764	L592	1765	L593	1766	L594	1767	L595	1768	L596	1769	L597	1770	L598	1771	L599	1772	L600	1773	L601	1774	L602	1775	L603	1776	L604	1777	L605	1778	L606	1779	L607	1780	L608	1781	L609	1782	L610	1783	L611	1784	L612	1785	L613	1786	L614	L615	1787	L616	1788	L617	L618	1789	L619	1790	L620	1791	L621	1792	L622	1793	L623	1794	L624	1795	L625	1796	L626	1797	L627	1798	L628	1799	L629	1800	L630	1801	L631	1802	L632	1803	L633	1804	L634	1805	L635	1806	L636	1807	L637	1808	L638	1809	L639	1810	L640	1811	L641	1812	L642	1813	L643	1814	L644	1815	L645	1816	L646	1817	L647	1818	L648	1819	L649	1820	L650	1821	L651	1822	L652	1823	L653	1824	L654	1825	L655	1826	L656	1827	L657	1828	L658	1829	L659	1830	L660	1831	L661	1832	L662	1833	L663	1834	L664	1835	L665	1836	L666	1837	L667	1838	L668	1839	L669	1840	L670	1841	L671	1842	L672	1843	L673	1844	L674	1845	L675	1846	L676	1847	L677	1848	L678	1849	L679	1850	L680	1851	L681	1852	L682	1853	L683	1854	L684	1855	L685	1856	L686	1857	L687	1858	L688	1859	L689	1860	L690	1861	L691	1862	L693	1863	L694	1864	L695	1865	L696	1866	L697	1867	L698	1868	L699	1869	L700	1870	L701	1871	L702	1872	L703	1873	L704	1874	L705	1875	L706	1876	L707	1877	L708	1878	L709	1879	L710	1880	L711	1881	1882	1883	1884	1885	1886	1887	1888	1889	1890	1891	1892	1893	1894	1895	1896	1897	1898	1899	1900	1901	1902	1903	1904	1905	1906	1907	1908	1909	1910	1911	1912	1913	1914	1915	1916	1917	1918	1919	1920	1921	1922	1923	1924	1925	1926	1927	1928	1929	1930	1931	1932	1933	1934	1935	1936	1937	1938	1939	1940	1941	1942	1943	1944	1945	1946	1947	1948	1949	1950	1951	1952	1953	1954	1955	1956	1957	1958	1959	1960	1961	1962	1963	1964	1965	1966	1967	1968	1969	1970	1971	1972	1973	1974	1975	1976	1977	1978	1979	1980	1981	1982	1983	1984	1985	1986	1987	1988	1989	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000
------	-----	------	-----	------	-----	------	-----	------	-----	------	-----	------	-----	------	-----	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	------	-----	------	-----	------	-----	------	-----	------	------	------	------	------	------	------	------	------	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

• Molecule 1: mu-like calpain



Y835	F661
S836	D662
M837	M663
I838	F664
I839	V665
R840	R666
ARG	C667
TYR	L668
S843	V669
G847	R670
N848	L671
M849	E672
D850	I673
F851	L674
N853	F675
F854	I677
I855	F678
S856	K679
S857	Q680
L858	L681
V859	D682
R860	P683
D862	E684
A863	M685
M864	T686
F865	G687
R866	T688
A867	I689
F868	Q690
R869	L691
S870	D692
L871	L693
D872	I694
K873	S695
N874	W696
G875	L697
T876	S698
G877	F699
Q878	S700
I879	V701
V880	L702
N881	GLY
N882	LYS
I883	LEU
Q884	ALA
E885	LYS
W886	ALA
L887	ALA
Q888	ALA
L889	ALA
T890	ALA
M891	ALA
Y892	ALA
S893	ALA
N714	LYS
I1E	LYS
GLU	LYS
ALA	LYS
N718	LYS
E719	LYS
S720	LYS
E0	LYS
GLU	LYS
E723	LYS
R724	LYS
Q725	LYS
F726	LYS
R727	LYS
K728	LYS
L729	LYS
F730	LYS
V731	LYS
F732	LYS
L733	LYS
ALA	LYS
GLY	LYS
ASP	LYS
ASP	LYS
ASP	LYS
M738	LYS
E739	LYS
V740	LYS
S741	LYS
A742	LYS
T743	LYS
E744	LYS
L745	LYS
M746	LYS
ASN	LYS
I1E	LYS
LEU	LYS
ASN	LYS
LYS	LYS
VAL	LYS
VAL	LYS
THR	LYS
THR	LYS
ARG	LYS
HIS	LYS
PRO	LYS
ASP	LYS
LEU	LYS
LEU	LYS
ALA	LYS
LYS	LYS
THR	LYS
ASP	LYS
GLY	LYS
F764	LYS
G765	LYS
I766	LYS
D767	LYS
H829	LYS
T768	LYS
C769	LYS
R770	LYS
M710	LYS
H711	LYS
Y712	LYS
M772	LYS
Y773	LYS
A774	LYS
V775	LYS
M776	LYS
D777	LYS
S778	LYS
D779	LYS
T780	LYS
T781	LYS
L784	LYS
G785	LYS
F786	LYS
E787	LYS
E788	LYS
F789	LYS
K790	LYS
Y791	LYS
L792	LYS
W793	LYS
M794	LYS
M795	LYS
I796	LYS
K797	LYS
K798	LYS
W799	LYS
Q800	LYS
G801	LYS
I802	LYS
TYR	LYS
LNS	LYS
R805	LYS
F806	LYS
E807	LYS
D808	LYS
R810	LYS
S811	LYS
G812	LYS
THR	LYS
I1E	LYS
GLY	LYS
SER	LYS
ASN	LYS
GLU	LYS
LEU	LYS
P820	LYS
G821	LYS
A822	LYS
F823	LYS
E824	LYS
A825	LYS
A826	LYS
G827	LYS
F828	LYS
H829	LYS
L830	LYS
M831	LYS
Q832	LYS
H833	LYS
I834	LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.74Å 184.60Å 86.37Å 90.00° 100.74° 90.00°	Depositor
Resolution (Å)	91.29 – 2.80 49.81 – 2.69	Depositor EDS
% Data completeness (in resolution range)	91.6 (91.29-2.80) 87.3 (49.81-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.229 , 0.311 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	55.6	Xtrriage
Anisotropy	0.074	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 98.8	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Outliers	0 of 55542 reflections	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12368	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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 [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	3.70	964/6177 (15.6%)	2.67	470/8354 (5.6%)
1	B	3.71	932/6128 (15.2%)	2.67	489/8288 (5.9%)
All	All	3.70	1896/12305 (15.4%)	2.67	959/16642 (5.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	45
1	B	0	39
All	All	0	84

The worst 5 of 1896 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	SER	CA-CB	28.73	1.96	1.52
1	A	339	GLU	CD-OE1	23.66	1.51	1.25
1	A	320	GLU	CD-OE2	20.06	1.47	1.25
1	B	429	GLU	CD-OE1	19.54	1.47	1.25
1	A	811	SER	CA-CB	-18.37	1.25	1.52

The worst 5 of 959 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ARG	NE-CZ-NH1	-29.77	105.41	120.30
1	A	329	ARG	NE-CZ-NH1	26.14	133.37	120.30
1	A	329	ARG	NE-CZ-NH2	-24.17	108.22	120.30
1	B	514	ASP	CB-CG-OD2	-18.56	101.59	118.30
1	A	285	ARG	NE-CZ-NH2	-15.96	112.32	120.30

There are no chirality outliers.

5 of 84 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ILE	Mainchain
1	A	152	VAL	Mainchain
1	A	24	ALA	Mainchain
1	A	29	ASN	Mainchain
1	A	99	GLN	Mainchain,Peptide

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	6053	0	5615	959	3
1	B	6003	0	5477	969	1
2	A	172	0	0	53	1
2	B	140	0	0	45	1
All	All	12368	0	11092	1928	3

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 83.

The worst 5 of 1928 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:583:VAL:CB	1:A:583:VAL:CA	1.74	1.65
1:B:0:GLU:CA	1:B:0:GLU:CB	1.75	1.64
1:B:786:PHE:CA	1:B:786:PHE:CB	1.74	1.64
1:A:550:ILE:CB	1:A:550:ILE:CA	1.75	1.64
1:B:8:LEU:CD2	1:B:8:LEU:CG	1.76	1.63

All (3) 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:457:ASN:OD1	2:B:1033:HOH:O[1_454]	1.56	0.64
1:A:442:LEU:CD2	2:A:922:HOH:O[1_455]	1.95	0.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASN:OD1	1:B:303:GLU:N[2_656]	2.08	0.12

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	747/900 (83%)	500 (67%)	143 (19%)	104 (14%)	0 1
1	B	748/900 (83%)	497 (66%)	146 (20%)	105 (14%)	0 1
All	All	1495/1800 (83%)	997 (67%)	289 (19%)	209 (14%)	0 1

5 of 209 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	60	PHE
1	A	63	LEU
1	A	67	SER
1	A	83	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	606/782 (78%)	459 (76%)	147 (24%)	1 2
1	B	584/782 (75%)	429 (74%)	155 (26%)	0 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1190/1564 (76%)	888 (75%)	302 (25%)	1 2

5 of 302 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	853	ASN
1	B	111	ILE
1	B	701	VAL
1	A	874	ASN
1	B	41	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	853	ASN
1	B	47	GLN
1	B	646	GLN
1	A	878	GLN
1	A	888	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 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, 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	783/900 (87%)	-0.35	5 (0%) 90 86	16, 49, 81, 98	0
1	B	788/900 (87%)	-0.32	11 (1%) 78 69	17, 51, 84, 102	0
All	All	1571/1800 (87%)	-0.33	16 (1%) 84 77	16, 50, 83, 102	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	587	ASP	3.8
1	B	596	LEU	3.8
1	A	596	LEU	3.4
1	B	712	TYR	3.3
1	B	402	SER	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 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.