



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2017 – 12:29 AM EDT

PDB ID : 5U7G  
Title : Crystal Structure of the Catalytic Core of CBP  
Authors : Park, S.; Stanfield, R.L.; Martinez-Yamout, M.M.; Dyson, H.J.; Wilson, I.A.; Wright, P.E.  
Deposited on : unknown  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20029824

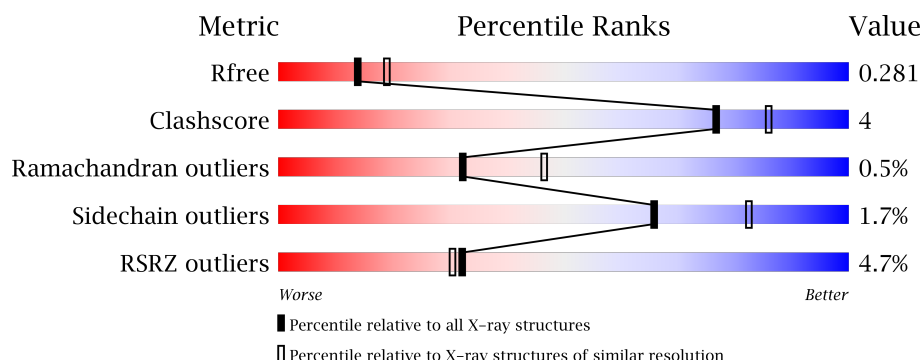
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	621	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 78%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> </div> </div>
1	B	621	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 79%; height: 10px; background-color: green;"></div> <div style="width: 9%; height: 10px; background-color: yellow;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8905 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 CREB-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4426	2836	749	806	35			
1	B	547	Total	C	N	O	S	0	0	0
			4426	2836	749	806	35			

There are 286 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1074	GLY	-	expression tag	UNP Q8QZV8
A	1075	ALA	-	expression tag	UNP Q8QZV8
A	1076	MET	-	expression tag	UNP Q8QZV8
A	1077	GLY	-	expression tag	UNP Q8QZV8
A	1078	SER	-	expression tag	UNP Q8QZV8
A	1557	SER	-	expression tag	UNP Q8QZV8
A	1558	GLY	-	expression tag	UNP Q8QZV8
A	1616	GLY	-	expression tag	UNP Q8QZV8
A	1617	SER	-	expression tag	UNP Q8QZV8
A	1618	GLY	-	expression tag	UNP Q8QZV8
A	1619	SER	-	expression tag	UNP Q8QZV8
A	1620	GLN	-	expression tag	UNP Q8QZV8
A	1621	LYS	-	expression tag	UNP Q8QZV8
A	1622	LEU	-	expression tag	UNP Q8QZV8
A	1623	TYR	-	expression tag	UNP Q8QZV8
A	1624	ALA	-	expression tag	UNP Q8QZV8
A	1625	THR	-	expression tag	UNP Q8QZV8
A	1626	MET	-	expression tag	UNP Q8QZV8
A	1627	GLU	-	expression tag	UNP Q8QZV8
A	1628	LYS	-	expression tag	UNP Q8QZV8
A	1629	HIS	-	expression tag	UNP Q8QZV8
A	1630	LYS	-	expression tag	UNP Q8QZV8
A	1631	GLU	-	expression tag	UNP Q8QZV8
A	1632	VAL	-	expression tag	UNP Q8QZV8
A	1633	PHE	-	expression tag	UNP Q8QZV8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1634	PHE	-	expression tag	UNP Q8QZV8
A	1635	VAL	-	expression tag	UNP Q8QZV8
A	1636	ILE	-	expression tag	UNP Q8QZV8
A	1637	HIS	-	expression tag	UNP Q8QZV8
A	1638	LEU	-	expression tag	UNP Q8QZV8
A	1639	HIS	-	expression tag	UNP Q8QZV8
A	1640	ALA	-	expression tag	UNP Q8QZV8
A	1641	GLY	-	expression tag	UNP Q8QZV8
A	1642	PRO	-	expression tag	UNP Q8QZV8
A	1643	VAL	-	expression tag	UNP Q8QZV8
A	1644	ILE	-	expression tag	UNP Q8QZV8
A	1645	SER	-	expression tag	UNP Q8QZV8
A	1646	THR	-	expression tag	UNP Q8QZV8
A	1647	GLN	-	expression tag	UNP Q8QZV8
A	1648	PRO	-	expression tag	UNP Q8QZV8
A	1649	PRO	-	expression tag	UNP Q8QZV8
A	1650	ILE	-	expression tag	UNP Q8QZV8
A	1651	VAL	-	expression tag	UNP Q8QZV8
A	1652	ASP	-	expression tag	UNP Q8QZV8
A	1653	PRO	-	expression tag	UNP Q8QZV8
A	1654	ASP	-	expression tag	UNP Q8QZV8
A	1655	PRO	-	expression tag	UNP Q8QZV8
A	1656	LEU	-	expression tag	UNP Q8QZV8
A	1657	LEU	-	expression tag	UNP Q8QZV8
A	1658	SER	-	expression tag	UNP Q8QZV8
A	1659	CYS	-	expression tag	UNP Q8QZV8
A	1660	ASP	-	expression tag	UNP Q8QZV8
A	1661	LEU	-	expression tag	UNP Q8QZV8
A	1662	MET	-	expression tag	UNP Q8QZV8
A	1663	ASP	-	expression tag	UNP Q8QZV8
A	1664	GLY	-	expression tag	UNP Q8QZV8
A	1665	ARG	-	expression tag	UNP Q8QZV8
A	1666	ASP	-	expression tag	UNP Q8QZV8
A	1667	ALA	-	expression tag	UNP Q8QZV8
A	1668	PHE	-	expression tag	UNP Q8QZV8
A	1669	LEU	-	expression tag	UNP Q8QZV8
A	1670	THR	-	expression tag	UNP Q8QZV8
A	1671	LEU	-	expression tag	UNP Q8QZV8
A	1672	ALA	-	expression tag	UNP Q8QZV8
A	1673	ARG	-	expression tag	UNP Q8QZV8
A	1674	ASP	-	expression tag	UNP Q8QZV8
A	1675	LYS	-	expression tag	UNP Q8QZV8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1676	HIS	-	expression tag	UNP Q8QZV8
A	1677	TRP	-	expression tag	UNP Q8QZV8
A	1678	GLU	-	expression tag	UNP Q8QZV8
A	1679	PHE	-	expression tag	UNP Q8QZV8
A	1680	SER	-	expression tag	UNP Q8QZV8
A	1681	SER	-	expression tag	UNP Q8QZV8
A	1682	LEU	-	expression tag	UNP Q8QZV8
A	1683	ARG	-	expression tag	UNP Q8QZV8
A	1684	ARG	-	expression tag	UNP Q8QZV8
A	1685	SER	-	expression tag	UNP Q8QZV8
A	1686	LYS	-	expression tag	UNP Q8QZV8
A	1687	TRP	-	expression tag	UNP Q8QZV8
A	1688	SER	-	expression tag	UNP Q8QZV8
A	1689	THR	-	expression tag	UNP Q8QZV8
A	1690	LEU	-	expression tag	UNP Q8QZV8
A	1691	CYS	-	expression tag	UNP Q8QZV8
A	1692	MET	-	expression tag	UNP Q8QZV8
A	1693	LEU	-	expression tag	UNP Q8QZV8
A	1694	VAL	-	expression tag	UNP Q8QZV8
A	1695	GLU	-	expression tag	UNP Q8QZV8
A	1696	LEU	-	expression tag	UNP Q8QZV8
A	1697	HIS	-	expression tag	UNP Q8QZV8
A	1698	THR	-	expression tag	UNP Q8QZV8
A	1699	GLN	-	expression tag	UNP Q8QZV8
A	1700	GLY	-	expression tag	UNP Q8QZV8
A	1701	GLN	-	expression tag	UNP Q8QZV8
A	1702	ASP	-	expression tag	UNP Q8QZV8
A	1703	ARG	-	expression tag	UNP Q8QZV8
A	1704	PHE	-	expression tag	UNP Q8QZV8
A	1705	VAL	-	expression tag	UNP Q8QZV8
A	1706	TYR	-	expression tag	UNP Q8QZV8
A	1707	THR	-	expression tag	UNP Q8QZV8
A	1708	CYS	-	expression tag	UNP Q8QZV8
A	1709	ASN	-	expression tag	UNP Q8QZV8
A	1710	GLU	-	expression tag	UNP Q8QZV8
A	1711	CYS	-	expression tag	UNP Q8QZV8
A	1712	LYS	-	expression tag	UNP Q8QZV8
A	1713	HIS	-	expression tag	UNP Q8QZV8
A	1714	HIS	-	expression tag	UNP Q8QZV8
A	1715	VAL	-	expression tag	UNP Q8QZV8
A	1716	GLU	-	expression tag	UNP Q8QZV8
A	1717	THR	-	expression tag	UNP Q8QZV8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1718	ARG	-	expression tag	UNP Q8QZV8
A	1719	TRP	-	expression tag	UNP Q8QZV8
A	1720	HIS	-	expression tag	UNP Q8QZV8
A	1721	CYS	-	expression tag	UNP Q8QZV8
A	1722	THR	-	expression tag	UNP Q8QZV8
A	1723	VAL	-	expression tag	UNP Q8QZV8
A	1724	CYS	-	expression tag	UNP Q8QZV8
A	1725	GLU	-	expression tag	UNP Q8QZV8
A	1726	ASP	-	expression tag	UNP Q8QZV8
A	1727	TYR	-	expression tag	UNP Q8QZV8
A	1728	ASP	-	expression tag	UNP Q8QZV8
A	1729	LEU	-	expression tag	UNP Q8QZV8
A	1730	CYS	-	expression tag	UNP Q8QZV8
A	1731	ILE	-	expression tag	UNP Q8QZV8
A	1732	ASN	-	expression tag	UNP Q8QZV8
A	1733	CYS	-	expression tag	UNP Q8QZV8
A	1734	TYR	-	expression tag	UNP Q8QZV8
A	1735	ASN	-	expression tag	UNP Q8QZV8
A	1736	THR	-	expression tag	UNP Q8QZV8
A	1737	LYS	-	expression tag	UNP Q8QZV8
A	1738	SER	-	expression tag	UNP Q8QZV8
A	1739	HIS	-	expression tag	UNP Q8QZV8
A	1740	THR	-	expression tag	UNP Q8QZV8
A	1741	HIS	-	expression tag	UNP Q8QZV8
A	1742	LYS	-	expression tag	UNP Q8QZV8
A	1743	MET	-	expression tag	UNP Q8QZV8
A	1744	VAL	-	expression tag	UNP Q8QZV8
A	1745	LYS	-	expression tag	UNP Q8QZV8
A	1746	TRP	-	expression tag	UNP Q8QZV8
A	1747	GLY	-	expression tag	UNP Q8QZV8
A	1748	LEU	-	expression tag	UNP Q8QZV8
A	1749	GLY	-	expression tag	UNP Q8QZV8
A	1750	LEU	-	expression tag	UNP Q8QZV8
A	1751	ASP	-	expression tag	UNP Q8QZV8
B	1074	GLY	-	expression tag	UNP Q8QZV8
B	1075	ALA	-	expression tag	UNP Q8QZV8
B	1076	MET	-	expression tag	UNP Q8QZV8
B	1077	GLY	-	expression tag	UNP Q8QZV8
B	1078	SER	-	expression tag	UNP Q8QZV8
B	1557	SER	-	expression tag	UNP Q8QZV8
B	1558	GLY	-	expression tag	UNP Q8QZV8
B	1616	GLY	-	expression tag	UNP Q8QZV8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1617	SER	-	expression tag	UNP Q8QZV8
B	1618	GLY	-	expression tag	UNP Q8QZV8
B	1619	SER	-	expression tag	UNP Q8QZV8
B	1620	GLN	-	expression tag	UNP Q8QZV8
B	1621	LYS	-	expression tag	UNP Q8QZV8
B	1622	LEU	-	expression tag	UNP Q8QZV8
B	1623	TYR	-	expression tag	UNP Q8QZV8
B	1624	ALA	-	expression tag	UNP Q8QZV8
B	1625	THR	-	expression tag	UNP Q8QZV8
B	1626	MET	-	expression tag	UNP Q8QZV8
B	1627	GLU	-	expression tag	UNP Q8QZV8
B	1628	LYS	-	expression tag	UNP Q8QZV8
B	1629	HIS	-	expression tag	UNP Q8QZV8
B	1630	LYS	-	expression tag	UNP Q8QZV8
B	1631	GLU	-	expression tag	UNP Q8QZV8
B	1632	VAL	-	expression tag	UNP Q8QZV8
B	1633	PHE	-	expression tag	UNP Q8QZV8
B	1634	PHE	-	expression tag	UNP Q8QZV8
B	1635	VAL	-	expression tag	UNP Q8QZV8
B	1636	ILE	-	expression tag	UNP Q8QZV8
B	1637	HIS	-	expression tag	UNP Q8QZV8
B	1638	LEU	-	expression tag	UNP Q8QZV8
B	1639	HIS	-	expression tag	UNP Q8QZV8
B	1640	ALA	-	expression tag	UNP Q8QZV8
B	1641	GLY	-	expression tag	UNP Q8QZV8
B	1642	PRO	-	expression tag	UNP Q8QZV8
B	1643	VAL	-	expression tag	UNP Q8QZV8
B	1644	ILE	-	expression tag	UNP Q8QZV8
B	1645	SER	-	expression tag	UNP Q8QZV8
B	1646	THR	-	expression tag	UNP Q8QZV8
B	1647	GLN	-	expression tag	UNP Q8QZV8
B	1648	PRO	-	expression tag	UNP Q8QZV8
B	1649	PRO	-	expression tag	UNP Q8QZV8
B	1650	ILE	-	expression tag	UNP Q8QZV8
B	1651	VAL	-	expression tag	UNP Q8QZV8
B	1652	ASP	-	expression tag	UNP Q8QZV8
B	1653	PRO	-	expression tag	UNP Q8QZV8
B	1654	ASP	-	expression tag	UNP Q8QZV8
B	1655	PRO	-	expression tag	UNP Q8QZV8
B	1656	LEU	-	expression tag	UNP Q8QZV8
B	1657	LEU	-	expression tag	UNP Q8QZV8
B	1658	SER	-	expression tag	UNP Q8QZV8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1659	CYS	-	expression tag	UNP Q8QZV8
B	1660	ASP	-	expression tag	UNP Q8QZV8
B	1661	LEU	-	expression tag	UNP Q8QZV8
B	1662	MET	-	expression tag	UNP Q8QZV8
B	1663	ASP	-	expression tag	UNP Q8QZV8
B	1664	GLY	-	expression tag	UNP Q8QZV8
B	1665	ARG	-	expression tag	UNP Q8QZV8
B	1666	ASP	-	expression tag	UNP Q8QZV8
B	1667	ALA	-	expression tag	UNP Q8QZV8
B	1668	PHE	-	expression tag	UNP Q8QZV8
B	1669	LEU	-	expression tag	UNP Q8QZV8
B	1670	THR	-	expression tag	UNP Q8QZV8
B	1671	LEU	-	expression tag	UNP Q8QZV8
B	1672	ALA	-	expression tag	UNP Q8QZV8
B	1673	ARG	-	expression tag	UNP Q8QZV8
B	1674	ASP	-	expression tag	UNP Q8QZV8
B	1675	LYS	-	expression tag	UNP Q8QZV8
B	1676	HIS	-	expression tag	UNP Q8QZV8
B	1677	TRP	-	expression tag	UNP Q8QZV8
B	1678	GLU	-	expression tag	UNP Q8QZV8
B	1679	PHE	-	expression tag	UNP Q8QZV8
B	1680	SER	-	expression tag	UNP Q8QZV8
B	1681	SER	-	expression tag	UNP Q8QZV8
B	1682	LEU	-	expression tag	UNP Q8QZV8
B	1683	ARG	-	expression tag	UNP Q8QZV8
B	1684	ARG	-	expression tag	UNP Q8QZV8
B	1685	SER	-	expression tag	UNP Q8QZV8
B	1686	LYS	-	expression tag	UNP Q8QZV8
B	1687	TRP	-	expression tag	UNP Q8QZV8
B	1688	SER	-	expression tag	UNP Q8QZV8
B	1689	THR	-	expression tag	UNP Q8QZV8
B	1690	LEU	-	expression tag	UNP Q8QZV8
B	1691	CYS	-	expression tag	UNP Q8QZV8
B	1692	MET	-	expression tag	UNP Q8QZV8
B	1693	LEU	-	expression tag	UNP Q8QZV8
B	1694	VAL	-	expression tag	UNP Q8QZV8
B	1695	GLU	-	expression tag	UNP Q8QZV8
B	1696	LEU	-	expression tag	UNP Q8QZV8
B	1697	HIS	-	expression tag	UNP Q8QZV8
B	1698	THR	-	expression tag	UNP Q8QZV8
B	1699	GLN	-	expression tag	UNP Q8QZV8
B	1700	GLY	-	expression tag	UNP Q8QZV8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1701	GLN	-	expression tag	UNP Q8QZV8
B	1702	ASP	-	expression tag	UNP Q8QZV8
B	1703	ARG	-	expression tag	UNP Q8QZV8
B	1704	PHE	-	expression tag	UNP Q8QZV8
B	1705	VAL	-	expression tag	UNP Q8QZV8
B	1706	TYR	-	expression tag	UNP Q8QZV8
B	1707	THR	-	expression tag	UNP Q8QZV8
B	1708	CYS	-	expression tag	UNP Q8QZV8
B	1709	ASN	-	expression tag	UNP Q8QZV8
B	1710	GLU	-	expression tag	UNP Q8QZV8
B	1711	CYS	-	expression tag	UNP Q8QZV8
B	1712	LYS	-	expression tag	UNP Q8QZV8
B	1713	HIS	-	expression tag	UNP Q8QZV8
B	1714	HIS	-	expression tag	UNP Q8QZV8
B	1715	VAL	-	expression tag	UNP Q8QZV8
B	1716	GLU	-	expression tag	UNP Q8QZV8
B	1717	THR	-	expression tag	UNP Q8QZV8
B	1718	ARG	-	expression tag	UNP Q8QZV8
B	1719	TRP	-	expression tag	UNP Q8QZV8
B	1720	HIS	-	expression tag	UNP Q8QZV8
B	1721	CYS	-	expression tag	UNP Q8QZV8
B	1722	THR	-	expression tag	UNP Q8QZV8
B	1723	VAL	-	expression tag	UNP Q8QZV8
B	1724	CYS	-	expression tag	UNP Q8QZV8
B	1725	GLU	-	expression tag	UNP Q8QZV8
B	1726	ASP	-	expression tag	UNP Q8QZV8
B	1727	TYR	-	expression tag	UNP Q8QZV8
B	1728	ASP	-	expression tag	UNP Q8QZV8
B	1729	LEU	-	expression tag	UNP Q8QZV8
B	1730	CYS	-	expression tag	UNP Q8QZV8
B	1731	ILE	-	expression tag	UNP Q8QZV8
B	1732	ASN	-	expression tag	UNP Q8QZV8
B	1733	CYS	-	expression tag	UNP Q8QZV8
B	1734	TYR	-	expression tag	UNP Q8QZV8
B	1735	ASN	-	expression tag	UNP Q8QZV8
B	1736	THR	-	expression tag	UNP Q8QZV8
B	1737	LYS	-	expression tag	UNP Q8QZV8
B	1738	SER	-	expression tag	UNP Q8QZV8
B	1739	HIS	-	expression tag	UNP Q8QZV8
B	1740	THR	-	expression tag	UNP Q8QZV8
B	1741	HIS	-	expression tag	UNP Q8QZV8
B	1742	LYS	-	expression tag	UNP Q8QZV8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1743	MET	-	expression tag	UNP Q8QZV8
B	1744	VAL	-	expression tag	UNP Q8QZV8
B	1745	LYS	-	expression tag	UNP Q8QZV8
B	1746	TRP	-	expression tag	UNP Q8QZV8
B	1747	GLY	-	expression tag	UNP Q8QZV8
B	1748	LEU	-	expression tag	UNP Q8QZV8
B	1749	GLY	-	expression tag	UNP Q8QZV8
B	1750	LEU	-	expression tag	UNP Q8QZV8
B	1751	ASP	-	expression tag	UNP Q8QZV8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	4	Total Zn 4 4	0	0
2	A	4	Total Zn 4 4	0	0

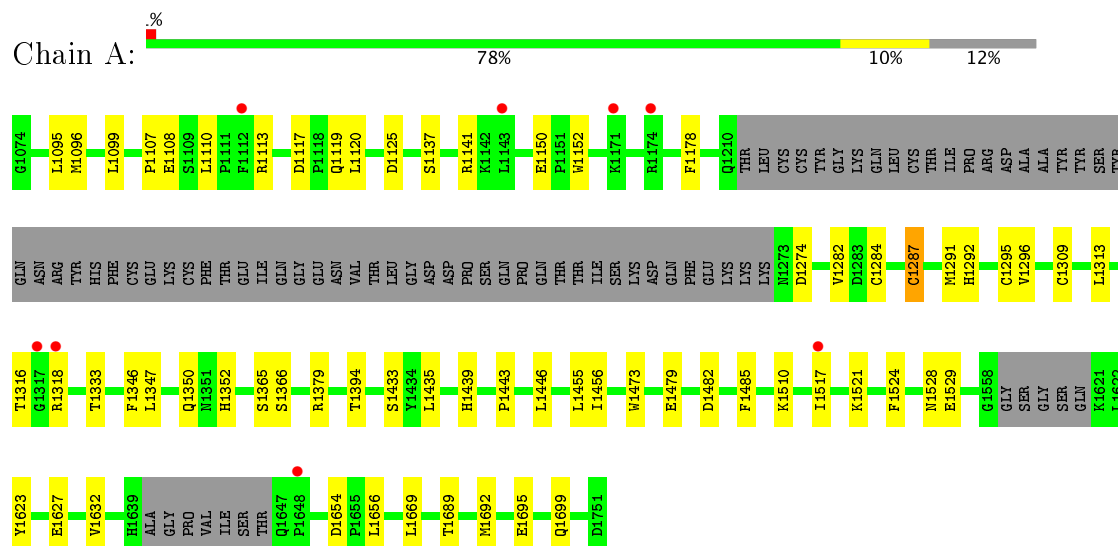
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	25	Total O 25 25	0	0
3	B	20	Total O 20 20	0	0

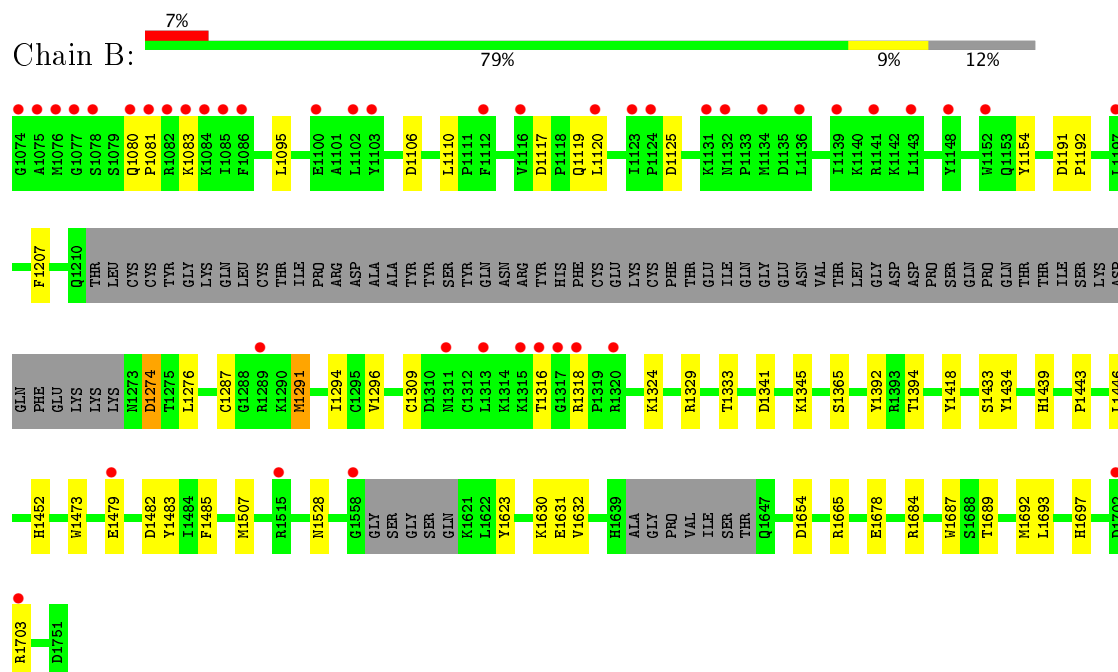
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: CREB-binding protein



#### • Molecule 1: CREB-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.17Å 87.17Å 114.98Å 90.00° 109.68° 90.00°	Depositor
Resolution (Å)	47.90 – 2.40 47.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.90-2.40) 92.2 (47.90-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, $R_{free}$	0.254 , 0.283 0.249 , 0.281	Depositor DCC
$R_{free}$ test set	3615 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8905	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.61 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.6861e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.56	1/4554 (0.0%)	0.65	0/6174
1	B	0.52	0/4554	0.62	0/6174
All	All	0.54	1/9108 (0.0%)	0.63	0/12348

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1287	CYS	CB-SG	-8.30	1.68	1.82

There are no bond angle outliers.

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	4426	0	4198	33	0
1	B	4426	0	4198	28	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	25	0	0	0	0
3	B	20	0	0	0	0
All	All	8905	0	8396	61	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 4.

All (61) 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:1689:THR:HA	1:B:1692:MET:HE3	1.68	0.73
1:B:1117:ASP:OD2	1:B:1120:LEU:HD13	1.93	0.68
1:A:1689:THR:HA	1:A:1692:MET:HE3	1.76	0.66
1:A:1528:ASN:OD1	1:A:1623:TYR:HE2	1.78	0.65
1:A:1117:ASP:OD2	1:A:1120:LEU:HD13	1.99	0.63
1:A:1291:MET:HG2	1:A:1296:VAL:HG11	1.81	0.62
1:B:1333:THR:HB	1:B:1654:ASP:OD2	2.06	0.56
1:A:1456:ILE:HD11	1:A:1510:LYS:HB3	1.87	0.55
1:B:1106:ASP:OD1	1:B:1110:LEU:HD21	2.06	0.55
1:A:1150:GLU:OE2	1:A:1152:TRP:HB2	2.08	0.54
1:A:1291:MET:HG2	1:A:1296:VAL:CG1	2.38	0.53
1:A:1113:ARG:O	1:A:1137:SER:HB3	2.10	0.51
1:B:1316:THR:HG22	1:B:1318:ARG:H	1.76	0.51
1:B:1434:TYR:CD2	1:B:1665:ARG:HD3	2.46	0.50
1:B:1365:SER:HA	1:B:1394:THR:O	2.12	0.50
1:B:1291:MET:HG2	1:B:1296:VAL:HG11	1.93	0.50
1:B:1294:ILE:HG23	1:B:1687:TRP:HB2	1.94	0.49
1:B:1678:GLU:OE1	1:B:1684:ARG:NH1	2.46	0.49
1:B:1392:TYR:HB3	1:B:1418:TYR:CD2	2.48	0.48
1:A:1443:PRO:HD2	1:A:1446:LEU:HD12	1.95	0.48
1:B:1482:ASP:HB3	1:B:1485:PHE:O	2.13	0.48
1:A:1435:LEU:HD11	1:A:1455:LEU:HD21	1.96	0.48
1:B:1528:ASN:OD1	1:B:1623:TYR:HE2	1.98	0.47
1:A:1333:THR:HB	1:A:1654:ASP:OD2	2.15	0.47
1:B:1630:LYS:HE3	1:B:1631:GLU:OE2	2.14	0.47
1:A:1695:GLU:OE2	1:A:1699:GLN:HG3	2.14	0.46
1:B:1392:TYR:HB3	1:B:1418:TYR:CE2	2.50	0.46
1:B:1443:PRO:HD2	1:B:1446:LEU:HD12	1.96	0.46
1:A:1352:HIS:CD2	1:A:1443:PRO:HG3	2.51	0.45
1:A:1524:PHE:CE1	1:A:1627:GLU:HB2	2.52	0.45
1:A:1365:SER:HA	1:A:1394:THR:O	2.18	0.44
1:B:1080:GLN:HG3	1:B:1083:LYS:HB2	1.98	0.44
1:A:1473:TRP:HD1	1:A:1632:VAL:HG12	1.82	0.44
1:B:1207:PHE:O	1:B:1276:LEU:HD22	2.18	0.44
1:B:1483:TYR:O	1:B:1665:ARG:HD2	2.17	0.44
1:A:1346:PHE:O	1:A:1350:GLN:HG2	2.18	0.43
1:B:1689:THR:HA	1:B:1692:MET:CE	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1292:HIS:HB2	1:A:1295:CYS:HB2	1.99	0.43
1:A:1521:LYS:HE2	1:A:1529:GLU:OE1	2.19	0.43
1:B:1083:LYS:HA	1:B:1287:CYS:O	2.19	0.42
1:B:1191:ASP:HB2	1:B:1192:PRO:HD3	2.01	0.42
1:B:1693:LEU:O	1:B:1697:HIS:HD2	2.01	0.42
1:A:1669:LEU:HA	1:A:1669:LEU:HD23	1.87	0.42
1:A:1096:MET:CE	1:A:1099:LEU:HD23	2.49	0.42
1:A:1347:LEU:HA	1:A:1347:LEU:HD23	1.85	0.42
1:A:1482:ASP:HB3	1:A:1485:PHE:O	2.20	0.42
1:A:1095:LEU:HA	1:A:1095:LEU:HD23	1.87	0.42
1:A:1316:THR:HG22	1:A:1318:ARG:H	1.84	0.42
1:A:1366:SER:HA	1:A:1656:LEU:HD22	2.02	0.41
1:B:1452:HIS:CD2	1:B:1507:MET:HB2	2.55	0.41
1:B:1324:LYS:O	1:B:1329:ARG:HD2	2.20	0.41
1:A:1108:GLU:HG3	1:A:1178:PHE:CD1	2.55	0.41
1:A:1517:ILE:HG21	1:A:1517:ILE:HD13	1.83	0.41
1:B:1341:ASP:O	1:B:1345:LYS:HB2	2.21	0.41
1:A:1473:TRP:CD1	1:A:1632:VAL:HG12	2.55	0.41
1:A:1099:LEU:HD12	1:A:1099:LEU:HA	1.88	0.41
1:A:1284:CYS:HB3	1:A:1287:CYS:HB2	2.02	0.40
1:B:1473:TRP:CD1	1:B:1632:VAL:HG12	2.56	0.40
1:B:1095:LEU:HD13	1:B:1154:TYR:CD2	2.57	0.40
1:A:1107:PRO:O	1:A:1110:LEU:HG	2.21	0.40
1:A:1313:LEU:O	1:A:1316:THR:HB	2.21	0.40

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	539/621 (87%)	518 (96%)	19 (4%)	2 (0%)	38 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	539/621 (87%)	518 (96%)	18 (3%)	3 (1%)	28	41
All	All	1078/1242 (87%)	1036 (96%)	37 (3%)	5 (0%)	32	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1274	ASP
1	B	1274	ASP
1	A	1479	GLU
1	B	1479	GLU
1	B	1081	PRO

### 5.3.2 Protein sidechains ⓘ

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	480/567 (85%)	472 (98%)	8 (2%)	66	82
1	B	480/567 (85%)	472 (98%)	8 (2%)	66	82
All	All	960/1134 (85%)	944 (98%)	16 (2%)	66	82

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1119	GLN
1	A	1125	ASP
1	A	1141	ARG
1	A	1282	VAL
1	A	1309	CYS
1	A	1379	ARG
1	A	1433	SER
1	A	1439	HIS
1	B	1119	GLN
1	B	1125	ASP
1	B	1274	ASP

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Mol	Chain	Res	Type
1	B	1291	MET
1	B	1309	CYS
1	B	1433	SER
1	B	1439	HIS
1	B	1703	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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

### 6.1 Protein, DNA and RNA chains

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	547/621 (88%)	-0.01	8 (1%) 74 72	29, 48, 80, 112	0
1	B	547/621 (88%)	0.39	43 (7%) 13 12	24, 56, 112, 149	0
All	All	1094/1242 (88%)	0.19	51 (4%) 32 30	24, 52, 101, 149	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1143	LEU	6.2
1	B	1317	GLY	5.7
1	B	1082	ARG	5.4
1	B	1080	GLN	5.3
1	B	1086	PHE	4.4
1	B	1081	PRO	4.2
1	B	1318	ARG	4.2
1	B	1315	LYS	4.1
1	B	1148	TYR	4.1
1	B	1558	GLY	4.0
1	B	1076	MET	3.9
1	B	1075	ALA	3.6
1	B	1141	ARG	3.3
1	B	1152	TRP	3.3
1	B	1074	GLY	3.2
1	B	1313	LEU	3.2
1	B	1085	ILE	3.1
1	A	1143	LEU	3.0
1	B	1116	VAL	3.0
1	B	1311	ASN	2.9
1	B	1102	LEU	2.9
1	B	1124	PRO	2.8
1	A	1171	LYS	2.8
1	B	1112	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1136	LEU	2.7
1	B	1132	ASN	2.7
1	A	1318	ARG	2.6
1	B	1316	THR	2.6
1	B	1131	LYS	2.6
1	B	1479	GLU	2.6
1	B	1515	ARG	2.5
1	A	1517	ILE	2.5
1	B	1703	ARG	2.4
1	B	1320	ARG	2.4
1	B	1289	ARG	2.4
1	B	1197	LEU	2.4
1	B	1702	ASP	2.3
1	B	1123	ILE	2.3
1	B	1083	LYS	2.3
1	B	1078	SER	2.2
1	A	1112	PHE	2.2
1	B	1077	GLY	2.2
1	A	1174	ARG	2.2
1	B	1103	TYR	2.2
1	B	1084	LYS	2.1
1	B	1139	ILE	2.1
1	B	1100	GLU	2.1
1	B	1134	MET	2.1
1	A	1317	GLY	2.1
1	A	1648	PRO	2.0
1	B	1120	LEU	2.0

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	B	1804	1/1	0.98	0.12	-0.93	58,58,58,58	0
2	ZN	B	1801	1/1	0.95	0.10	-1.02	55,55,55,55	0
2	ZN	A	1801	1/1	0.99	0.11	-1.24	33,33,33,33	0
2	ZN	A	1804	1/1	0.94	0.09	-1.49	71,71,71,71	0
2	ZN	A	1803	1/1	0.99	0.04	-2.06	45,45,45,45	0
2	ZN	B	1802	1/1	0.97	0.03	-2.26	71,71,71,71	0
2	ZN	B	1803	1/1	0.99	0.04	-	46,46,46,46	0
2	ZN	A	1802	1/1	0.98	0.07	-	48,48,48,48	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.