wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 11:11 AM EDT

PDB ID	:	1OD4
Title	:	Acetyl-CoA Carboxylase Carboxyltransferase Domain
Authors	:	Zhang, H.; Yang, Z.; Shen, Y.; Tong, L.
Deposited on	:	2003-02-12
Resolution	:	2.70 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

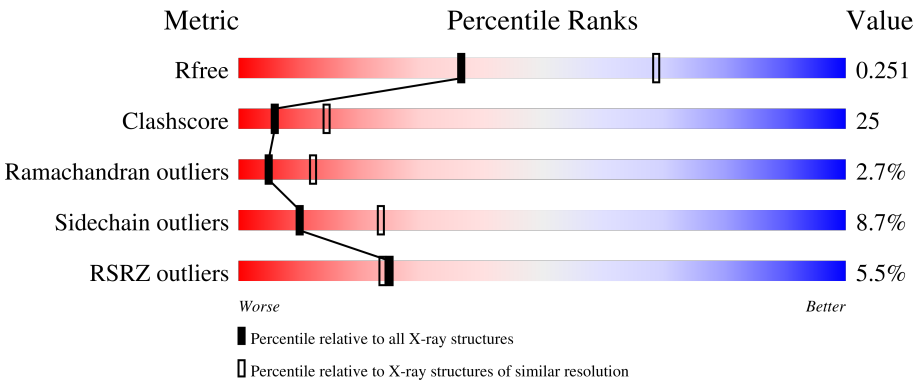
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	805	3%, 49%, 31%, 5%, 15%
1	B	805	6%, 46%, 34%, 5%, 15%
1	C	805	4%, 47%, 30%, 5% •, 17%

2 Entry composition (i)

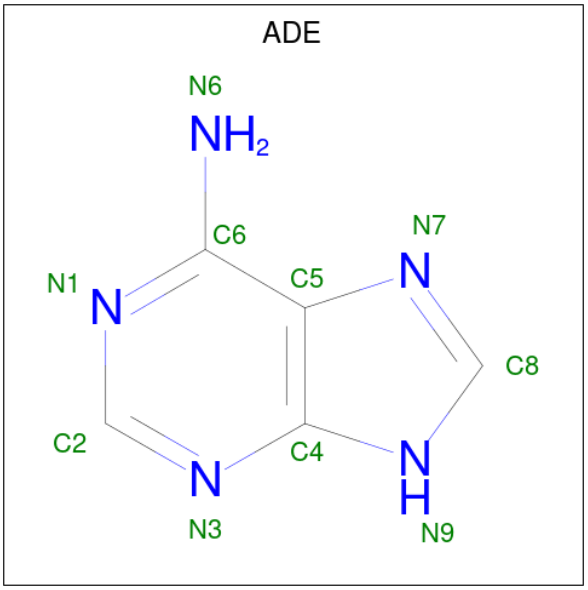
There are 3 unique types of molecules in this entry. The entry contains 16461 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-COENZYME A CARBOXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	684	5444	3471	936	1018	2	17	0	0	1
1	B	684	5444	3471	936	1018	2	17	0	0	1
1	C	672	5347	3406	920	1002	2	17	0	0	1

- Molecule 2 is ADENINE (three-letter code: ADE) (formula: $C_5H_5N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	C	1	10	5	5	0	0

- Molecule 3 is water.

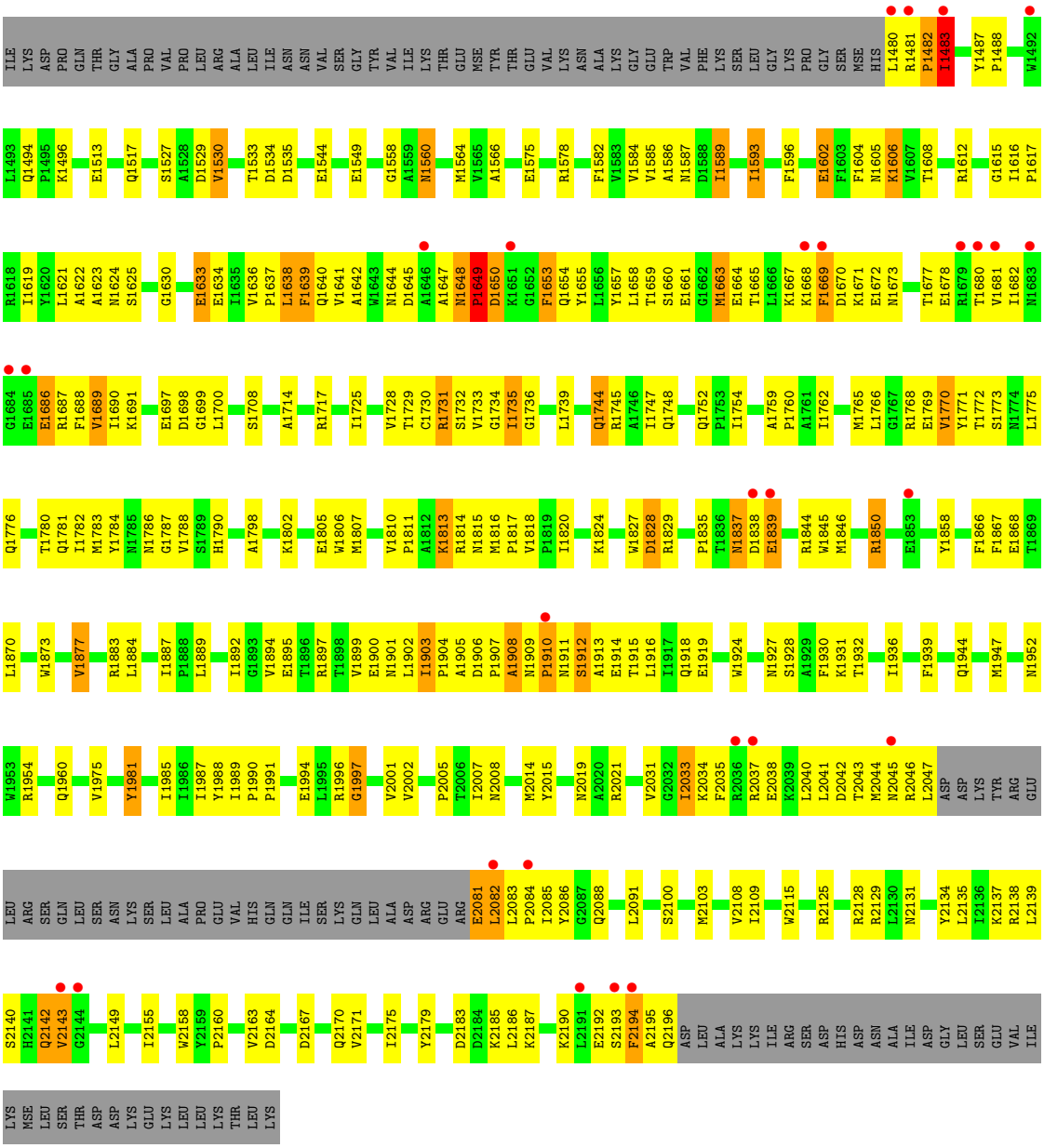
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	86	86	86	0	0
			Total	O		
3	B	70	70	70	0	0
			Total	O		
3	C	60	60	60	0	0

3 Residue-property plots (i)

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.

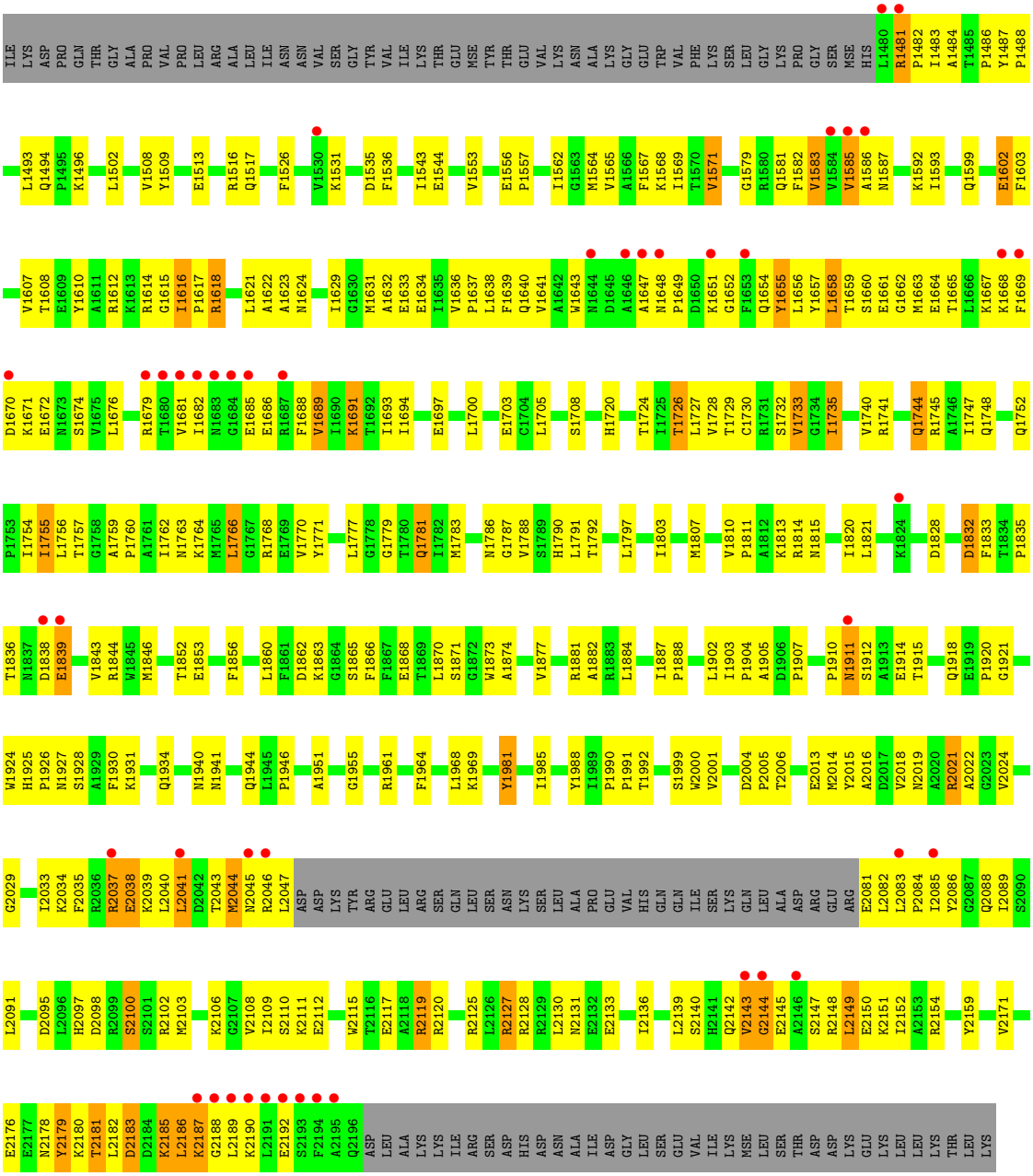
- Molecule 1: ACETYL-COENZYME A CARBOXYLASE

Chain A: 3% 49% 31% 5% 15%



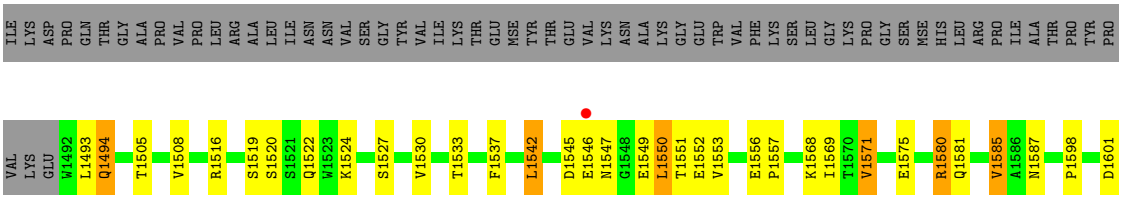
• Molecule 1: ACETYL-COENZYME A CARBOXYLASE

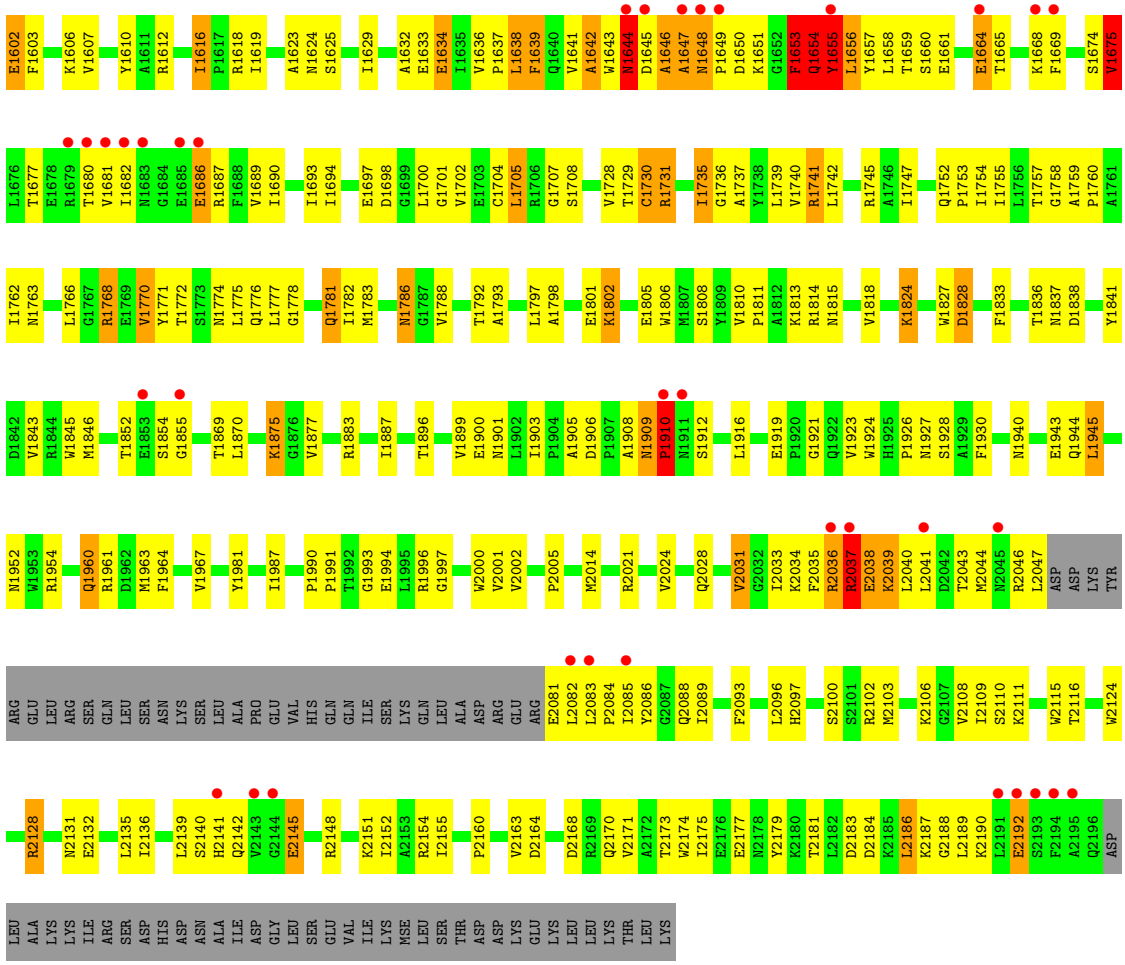
Chain B:



• Molecule 1: ACETYL-COENZYME A CARBOXYLASE

Chain C:




E1602 F1603 K1606 V1607 Y1610 A1611 R1612 I1616 P1617 R1618 I1619 A1623 N1624 S1625 I1629 A1632 E1633 E1634 I1635 V1636 P1637 L1638 F1639 Q1640 V1641 A1642 W1643 N1644 D1645 A1646 A1647 N1648 P1649 D1650 K1651 G1652 F1653 Q1654 Y1655 L1656 Y1657 L1658 T1659 S1660 E1661 E1664 T1665 K1668 F1669 S1674 Y1675
L1676 T1677 E1678 R1679 T1680 V1681 I1682 N1683 G1684 E1685 E1686 R1687 F1688 V1689 I1690 I1693 I1694 E1697 D1698 G1699 L1700 G1701 V1702 E1703 C1704 L1705 R1706 G1707 S1708 V1728 T1729 C1730 R1731 I1735 G1736 A1737 Y1738 L1739 V1740 R1741 L1742 R1745 A1746 I1747 Q1752 P1753 I1754 I1755 L1756 T1757 G1758 A1759 P1760 A1761
I1762 N1763 L1766 G1767 R1768 E1769 V1770 Y1771 T1772 S1773 N1774 L1775 Q1776 L1777 G1778 Q1781 I1782 M1783 N1786 G1787 V1788 T1792 A1793 L1797 A1798 E1801 K1802 E1805 W1806 H1807 S1808 Y1809 V1810 P1811 A1812 K1813 R1814 N1815 V1818 K1824 W1827 D1828 F1833 T1836 N1837 D1838 Y1841
D1842 V1843 R1844 W1845 M1846 T1852 E1853 S1854 G1855 T1869 L1870 K1875 G1876 V1877 R1883 I1887 T1896 V1899 E1900 N1901 L1902 I1903 P1904 A1905 D1906 P1907 A1908 N1909 P1910 N1911 S1912 L1916 E1919 P1920 G1921 Q1922 V1923 W1924 H1925 P1926 N1927 S1928 A1929 F1930 N1940 E1943 Q1944 L1945
N1952 W1953 R1954 Q1960 R1961 D1962 M1963 F1964 V1967 Y1981 I1987 P1990 P1991 T1992 G1993 E1994 L1995 R1996 G1997 W2000 V2001 V2002 P2005 M2014 R2021 V2024 Q2028 V2031 G2032 I2033 K2034 F2035 R2036 R2037 E2038 K2039 L2040 L2041 D2042 T2043 M2044 N2045 R2046 L2047 ASP ASP LYS TYR
ARG GLU LEU ARG SER GLN LEU SER ASN LYS SER LEU ALA PRO GLU VAL HIS GLN GLN ILE SER LYS GLN LEU ALA ASP ARG GLU ARG E2081 L2082 L2083 P2084 I2085 Y2086 G2087 Q2088 I2089 F2093 L2096 H2097 S2100 S2101 R2102 M2103 K2106 G2107 V2108 I2109 S2110 K2111 W2115 T2116 W2124
R2128 N2131 E2132 L2135 I2136 L2139 S2140 H2141 Q2142 V2143 G2144 E2145 R2148 K2151 I2152 A2153 R2154 I2155 P2160 V2163 D2164 D2168 R2169 Q2170 V2171 A2172 T2173 W2174 I2175 E2176 E2177 N2178 Y2179 K2180 T2181 L2182 D2183 D2184 K2185 L2186 K2187 G2188 L2189 K2190 L2191 E2192 S2193 F2194 A2195 Q2196 ASP
LEU ALA LYS LYS ILE ARG SER ASP HIS ASP ASN ALA ILE ASP GLY LEU SER GLU VAL ILE LYS MSE LEU SER THR ASP ASP LYS GLU LYS LEU LEU LYS THR LEU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	246.91Å 123.91Å 145.07Å 90.00° 94.11° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 28.94 – 2.69	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.70) 94.1 (28.94-2.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.44 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.262 0.218 , 0.251	Depositor DCC
R_{free} test set	11315 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16461	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ADE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.45	0/5549	0.68	1/7491 (0.0%)
1	B	0.46	0/5549	0.68	1/7491 (0.0%)
1	C	0.45	0/5448	0.67	2/7351 (0.0%)
All	All	0.45	0/16546	0.68	4/22333 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1912	SER	N-CA-C	-6.10	94.53	111.00
1	C	1644	ASN	N-CA-C	-5.58	95.95	111.00
1	C	1656	LEU	N-CA-C	-5.33	96.59	111.00
1	B	1912	SER	N-CA-C	-5.02	97.44	111.00

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	5444	0	5388	269	1
1	B	5444	0	5388	292	0
1	C	5347	0	5283	280	0
2	C	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	86	0	0	4	0
3	B	70	0	0	4	0
3	C	60	0	0	4	0
All	All	16461	0	16063	804	1

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 25.

The worst 5 of 804 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:1735:ILE:HD13	1:B:1735:ILE:H	1.06	1.21
1:B:1631:MSE:HE2	1:C:2034:LYS:HB3	1.35	1.09
1:C:2014:MSE:HE3	1:C:2109:ILE:HG22	1.36	1.08
1:A:1658:LEU:HD12	1:A:1663:MSE:HE1	1.40	1.03
1:C:1658:LEU:HG	1:C:1690:ILE:HD11	1.42	0.99

All (1) 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:1717:ARG:NH2	1:A:2007:ILE:O[2_555]	2.16	0.04

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	680/805 (84%)	589 (87%)	70 (10%)	21 (3%)	4 9
1	B	680/805 (84%)	602 (88%)	64 (9%)	14 (2%)	7 18
1	C	668/805 (83%)	582 (87%)	66 (10%)	20 (3%)	4 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2028/2415 (84%)	1773 (87%)	200 (10%)	55 (3%)	5 12

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1483	ILE
1	A	1530	VAL
1	A	1650	ASP
1	A	1839	GLU
1	B	2037	ARG

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	579/668 (87%)	534 (92%)	45 (8%)	12 29
1	B	579/668 (87%)	528 (91%)	51 (9%)	10 23
1	C	568/668 (85%)	513 (90%)	55 (10%)	8 19
All	All	1726/2004 (86%)	1575 (91%)	151 (9%)	10 23

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1651	LYS
1	C	2037	ARG
1	C	1664	GLU
1	C	1802	LYS
1	C	2192	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1640	GLN
1	C	2142	GLN

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Mol	Chain	Res	Type
1	C	1648	ASN
1	C	1909	ASN
1	A	2131	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADE	C	3196	-	9,11,11	1.59	2 (22%)	7,15,15	1.13	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADE	C	3196	-	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3196	ADE	C2-N3	3.18	1.37	1.32
2	C	3196	ADE	C4-N9	2.39	1.39	1.34

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 (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	667/805 (82%)	-0.05	28 (4%)	36	35	20, 36, 74, 88	0
1	B	667/805 (82%)	0.05	45 (6%)	17	16	21, 38, 77, 94	0
1	C	655/805 (81%)	0.02	36 (5%)	25	24	23, 39, 77, 92	0
All	All	1989/2415 (82%)	0.00	109 (5%)	25	24	20, 38, 76, 94	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1480	LEU	6.7
1	B	2143	VAL	6.5
1	B	2194	PHE	6.4
1	B	2191	LEU	6.3
1	C	2194	PHE	6.3

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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
2	ADE	C	3196	10/10	0.69	0.36	86,87,87,88	0

6.5 Other polymers (i)

There are no such residues in this entry.