



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:18 PM GMT

PDB ID : 1OD2
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
<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

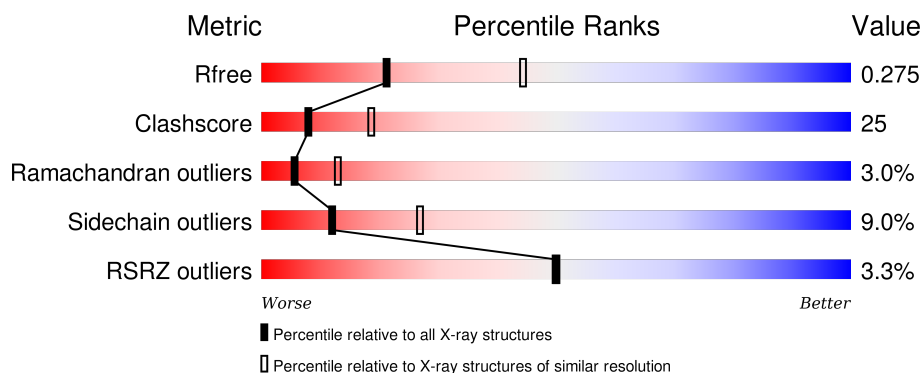
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 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	805	<div> <div>3%</div> <div>52%</div> <div>32%</div> <div>5%</div> <div>11%</div> </div>
1	B	805	<div> <div>2%</div> <div>44%</div> <div>37%</div> <div>5%</div> <div>14%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADE	B	3190	-	-	-	X

2 Entry composition [i](#)

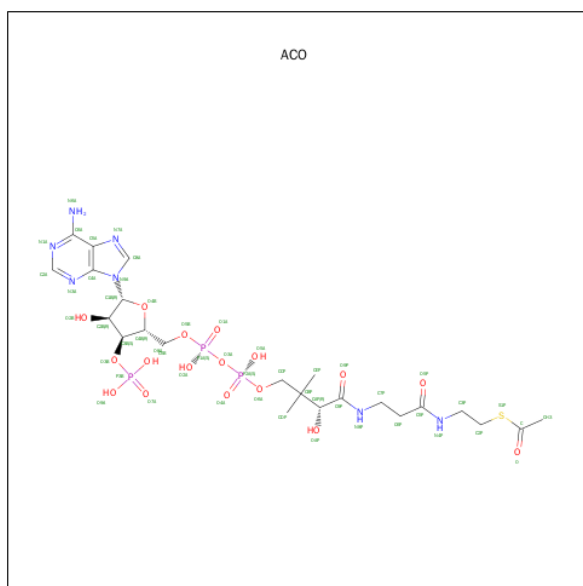
There are 4 unique types of molecules in this entry. The entry contains 11433 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

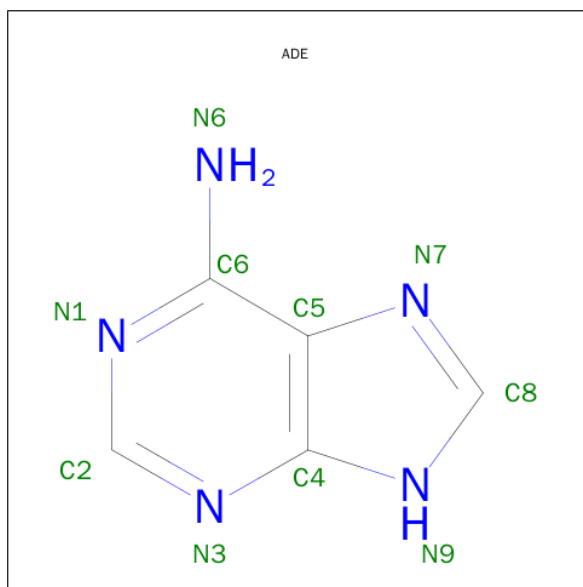
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	720	Total	C	N	O	S	Se	0	0	1
			5742	3650	994	1079	2	17			
1	B	696	Total	C	N	O	S	Se	0	0	1
			5544	3518	963	1044	2	17			

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is ADENINE (three-letter code: ADE) (formula: $C_5H_5N_5$).



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

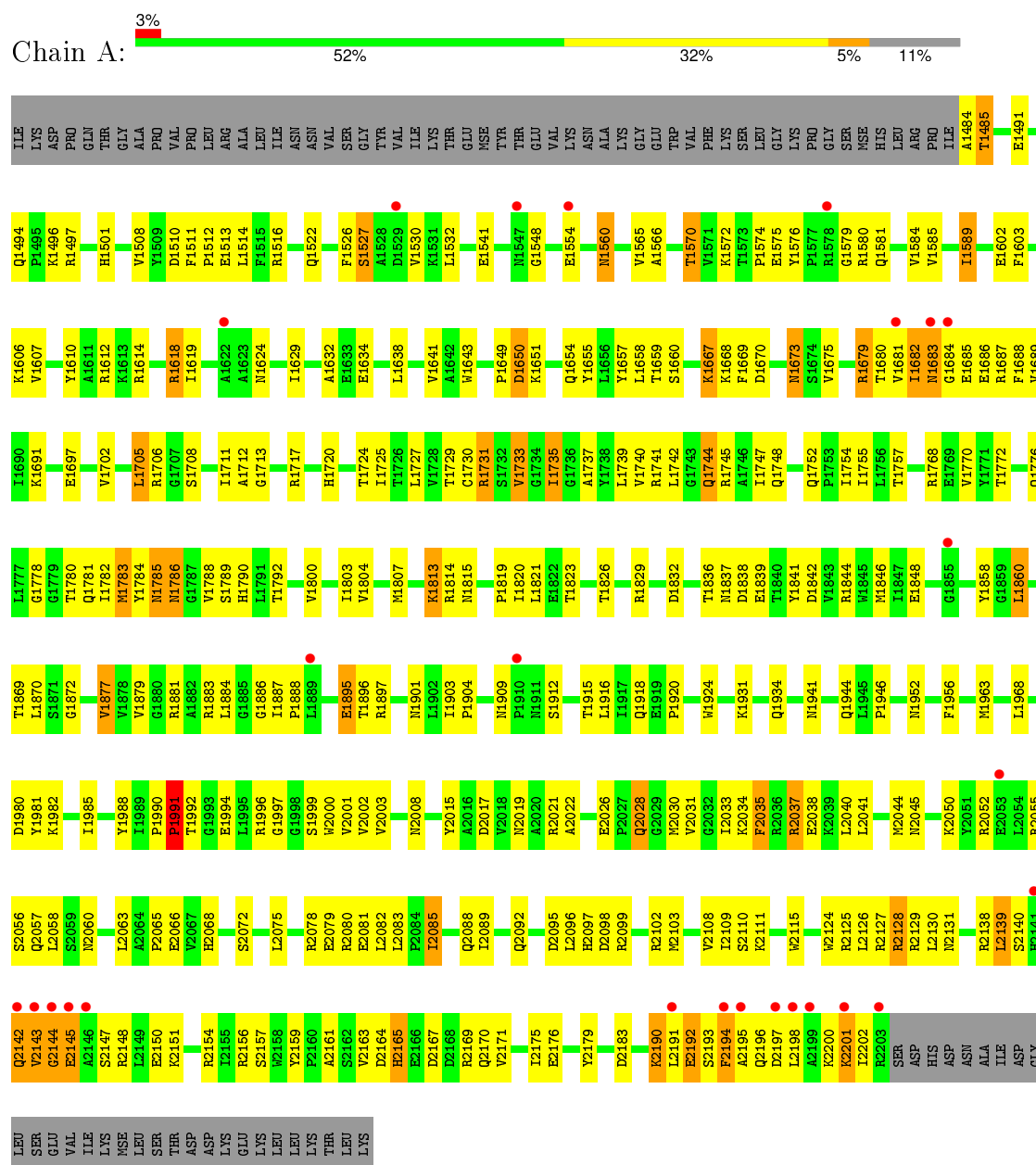
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	42	Total	O	0	0
			42	42		

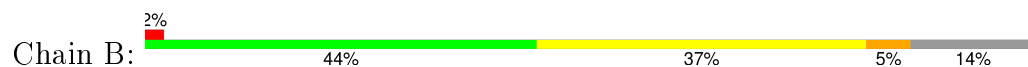
3 Residue-property plots

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: ACETYL-COENZYME A CARBOXYLASE



- Molecule 1: ACETYL-COENZYME A CARBOXYLASE



ILE	VAL	M1560	H1643	A1712	D1796	R1883	V1975	K2061	Q2142	ILE
LYS	LYS	F1567	M1644	G1713	L1797	I1887	V1979	S2062	V2143	ASP
PRO	TRP	K1568	D1645	R1717	E1801	V1891	D1980	L2063	G2144	GLY
GLN	GLN	I1569	A1646	R1725	E1807	V1895	K1982	A2064	E2145	LEU
THR	GLN	K1572	H1647	T1726	M1807	E1896	Q1983	V2067	S2146	SER
GLY	P1495	K1575	P1649	T1727	V1810	T1896	F1984	Q2070	R2148	VAL
ALA	K1496	E1575	D1650	V1728	P1811	R1897	I1985	I2071	L2149	ILE
PRO	R1497	K1498	K1651	C1729	A1812	L1902	I1986	Q2074	E2150	LYS
VAL	K1499	G1579	G1652	T1730	R1813	L1903	I1987	L2075	K2151	LEU
LEU	L1502	V1583	Q1654	S1732	H1815	P1904	P1990	A2076	A2153	SER
ARG	T1505	V1584	Y1655	V1733	M1816	A1905	F1991	D2077	R2154	THR
ALA	T1506	N1587	L1656	I1735	P1817	D1906	G1992	D2078	L2155	ASP
LEU	Y1507	N1588	T1659	L1739	V1818	P1910	L1994	E2079	W2158	ASP
ASN	Y1508	D1589	G1661	V1740	P1819	M1911	R1995	E2080	Y2159	GLY
VAL	E1513	T1590	E1662	R1741	I1820	S1912	G1997	L2081	P2160	LYS
SER	L1514	K1591	M1663	Q1744	W1827	A1913	G1998	L2082	V2163	LEU
GLY	F1515	K1592	F1591	I1747	D1828	E1914	S1999	L2083	D2164	LEU
TYR	R1516	I1593	E1664	Q1748	R1829	P1917	W2000	P2084	H2165	THR
VAL	Q1517	G1594	K1668	V1749	V1830	I1917	V2001	Z2085	E2166	LEU
LYS	W1523	P1598	F1669	I1756	P1831	G1921	D2010	Y2086	D2167	LYS
THR	F1526	Q1599	D1670	T1757	V1831	Q1922	Z2011	Q2087	D2168	
GLU	S1527	E1600	K1671	G1758	T1834	Q1923	M2011	Q2088	V2171	
THR	D1601	K1602	E1672	L1766	P1835	W1924	E2012	L2089	N2178	
GLU	D1529	K1606	S1674	L1768	T1836	H1925	M2013	S2090	Y2179	
VAL	V1530	V1607	V1675	R1768	N1837	P1926	R2021	L2091	K2180	
LYS	A1531	V1607	L1676	G1768	D1838	S1927	V2024	Q2092	T2181	
ASN	L1532	Y1610	T1679	A1759	E1839	S1928	L2025	E2097	L2182	
ALA	T1533	Y1681	V1681	P1760	V1843	Q1934	L2026	S2100	D2183	
LYS	D1534	G1615	I1682	M1765	R1844	A1935	E2027	M2103	D2184	
GLY	F1536	I1616	N1683	L1766	T1852	I1936	Q2028	K2106	K2185	
GLU	F1537	P1617	E1684	G1767	E1853	M1940	G2029	G2107	K2186	
TRP	I1538	R1618	E1685	R1768	S1854	M1947	F2035	V2108	G2187	
VAL	S1539	I1619	E1686	T1772	G1855	M1948	R2036	I2109	G2188	
PHE	N1540	L1621	R1687	S1773	F1856	L1949	R2037	R2119	L2189	
LYS	E1541	A1622	F1688	Q1776	L1860	L1950	E2038	R2125	K2190	
SER	L1542	A1623	V1689	G1779	K1863	A1951	L2040	L2126	LEU	
LEU	I1543	M1624	I1690	T1780	G1864	M1952	M2044	R2127	GLU	
GLY	D1544	S1625	K1691	Q1781	S1865	W1953	R2045	R2128	ALA	
PRO	D1545	G1626	I1694	I1782	L1870	G1955	R2046	R2129	LEU	
GLY	N1546	M1631	I1694	M1783	S1871	Q1960	L2047	L2130	ALA	
SER	G1548	A1632	D1698	Y1784	G1872	R1961	R2048	E2132	LYS	
MSE	E1549	E1632	G1699	N1785	W1873	D1962	L2047	L2135	ILE	
HIS	V1552	E1634	L1700	N1786	A1874	M1963	K2050	T2136	ARG	
LEU	E1553	P1637	G1701	V1702	V1877	E1966	R2051	K2137	SER	
ARG	E1554	L1638	V1703	E1703	V1878	E1967	R2052	R2138	ASP	
PRO	R1555	F1639	C1704	S1789	V1878	V1968	R2055	L2140	HIS	
ILE	E1556	Q1640	L1705	L1791	R1881	K1969	L2058	R2141	ASP	
ALA	E1557	V1641	I1711	T1792	A1882				ALA	
THR	G1558	A1559								
TYR										
PRO										

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.87Å 138.13Å 101.40Å 90.00° 114.42° 90.00°	Depositor
Resolution (Å)	28.85 – 2.70 28.85 – 2.69	Depositor EDS
% Data completeness (in resolution range)	93.2 (28.85-2.70) 92.7 (28.85-2.69)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.54 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.279 0.224 , 0.275	Depositor DCC
R_{free} test set	6032 reflections (11.27%)	DCC
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.4	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 60061 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11433	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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](#)

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

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	0/5850	0.66	0/7893
1	B	0.45	0/5646	0.67	0/7615
All	All	0.45	0/11496	0.66	0/15508

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 [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	5742	0	5688	271	0
1	B	5544	0	5483	318	0
2	A	48	0	31	4	0
3	B	10	0	4	0	0
4	A	47	0	0	1	0
4	B	42	0	0	2	0
All	All	11433	0	11206	558	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 25.

The worst 5 of 558 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:2085:ILE:HD12	1:A:2085:ILE:H	1.17	1.06
1:A:2085:ILE:HG12	1:B:1650:ASP:HA	1.38	1.01
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.18	0.99
1:A:2034:LYS:HB2	1:B:1631:MSE:HE3	1.48	0.96
1:B:1940:ASN:HD22	1:B:1983:GLN:HE22	1.07	0.94

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	718/805 (89%)	640 (89%)	61 (8%)	17 (2%)	7	19
1	B	694/805 (86%)	608 (88%)	61 (9%)	25 (4%)	4	9
All	All	1412/1610 (88%)	1248 (88%)	122 (9%)	42 (3%)	5	13

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1683	ASN
1	A	1991	PRO
1	A	2144	GLY
1	A	2194	PHE
1	B	1838	ASP

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	612/668 (92%)	556 (91%)	56 (9%)	11	25
1	B	591/668 (88%)	539 (91%)	52 (9%)	12	28
All	All	1203/1336 (90%)	1095 (91%)	108 (9%)	12	27

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2163	VAL
1	B	1540	ASN
1	B	2091	LEU
1	A	2179	TYR
1	A	2194	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2060	ASN
1	B	1525	ASN
1	B	2097	HIS
1	A	2131	ASN
1	B	1540	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are 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	ACO	A	3203	-	40,50,53	1.18	5 (12%)	50,75,79	1.87	9 (18%)
3	ADE	B	3190	-	8,11,11	1.47	2 (25%)	4,15,15	1.25	1 (25%)

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	ACO	A	3203	-	-	0/44/64/67	0/3/3/3
3	ADE	B	3190	-	-	0/0/0/0	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3203	ACO	C8A-N7A	-2.13	1.30	1.34
2	A	3203	ACO	CDP-CBP	2.01	1.58	1.53
2	A	3203	ACO	C9P-N8P	2.16	1.38	1.33
3	B	3190	ADE	C4-N9	2.36	1.39	1.34
2	A	3203	ACO	C4A-N3A	2.69	1.39	1.35

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3203	ACO	N3A-C2A-N1A	-4.25	125.64	128.89
2	A	3203	ACO	P2A-O3A-P1A	-4.15	121.08	132.73
2	A	3203	ACO	C2P-C3P-N4P	-3.92	104.64	112.37
2	A	3203	ACO	CDP-CBP-CCP	-2.30	105.52	108.50
3	B	3190	ADE	N3-C2-N1	-2.21	127.20	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3203	ACO	4	0

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	703/805 (87%)	0.02	26 (3%) 45 45	22, 37, 58, 74	0
1	B	679/805 (84%)	-0.01	19 (2%) 56 57	20, 38, 59, 69	0
All	All	1382/1610 (85%)	0.01	45 (3%) 50 50	20, 38, 59, 74	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2143	VAL	8.0
1	A	2194	PHE	5.2
1	A	2146	ALA	4.5
1	A	2203	ARG	4.4
1	A	2201	LYS	4.3

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](#)

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	ADE	B	3190	10/10	0.85	0.28	2.28	61,63,63,64	0
2	ACO	A	3203	48/51	0.91	0.17	-0.34	56,68,77,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.