



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 29, 2017 – 10:48 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](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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
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-20029077

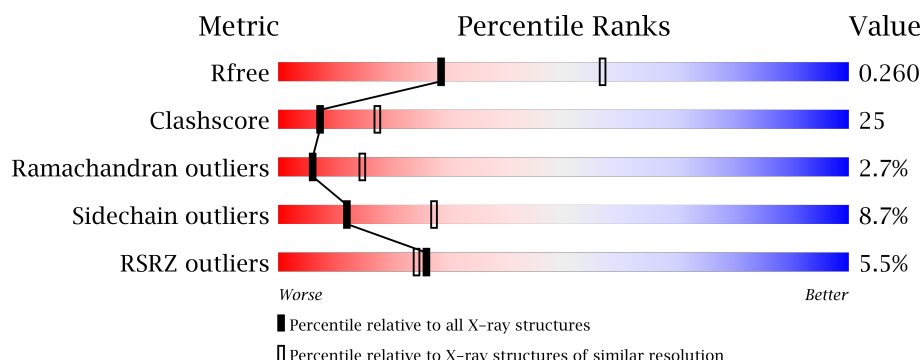
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (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  $\geq 3$ , 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	805	<div> <div>3%</div> <div>49%</div> <div>31%</div> <div>5%</div> <div>15%</div> </div>
1	B	805	<div> <div>6%</div> <div>46%</div> <div>34%</div> <div>5%</div> <div>15%</div> </div>
1	C	805	<div> <div>4%</div> <div>47%</div> <div>30%</div> <div>5%</div> <div>17%</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
2	ADE	C	3196	-	-	-	X

## 2 Entry composition [i](#)

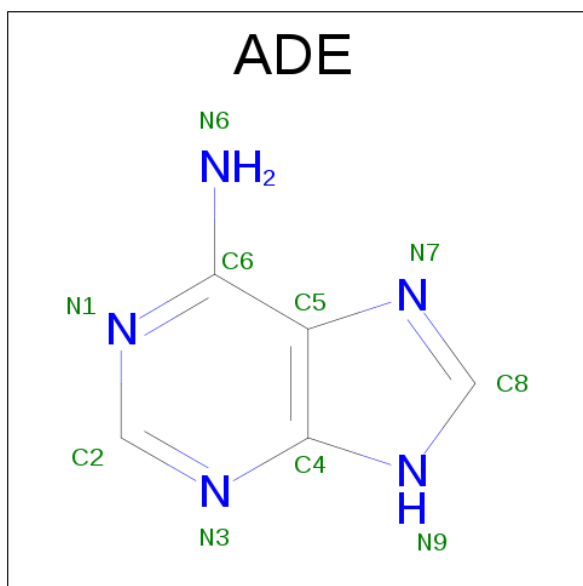
There are 3 unique types of molecules in this entry. The entry contains 16461 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	684	Total	C	N	O	S	Se	0	0	1
			5444	3471	936	1018	2	17			
1	B	684	Total	C	N	O	S	Se	0	0	1
			5444	3471	936	1018	2	17			
1	C	672	Total	C	N	O	S	Se	0	0	1
			5347	3406	920	1002	2	17			

- Molecule 2 is ADENINE (three-letter code: ADE) (formula: C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>).



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

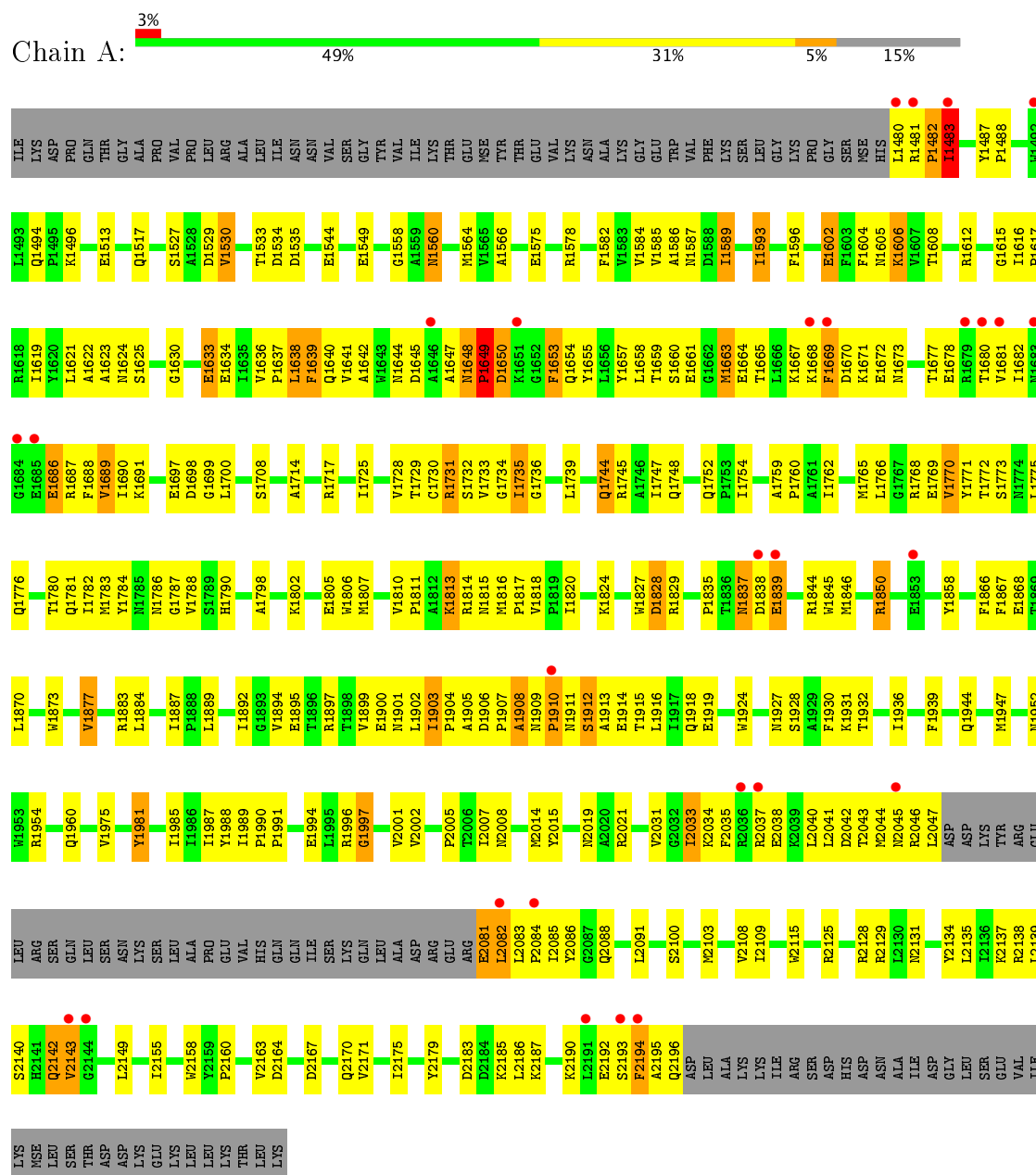
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total 86	O 86	0	0
3	B	70	Total 70	O 70	0	0
3	C	60	Total 60	O 60	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: ACETYL-COENZYME A CARBOXYLASE



- Molecule 1: ACETYL-COENZYME A CARBOXYLASE



ILE	L1493	V1607	D1670	P1753	T1836	H1924	G2029	L2091	E2176
LYS	L1494	T1608	K1671	I1754	M1837	H1925	K2033	D2095	E2177
ASP	P1495	E1609	E1672	I1756	E1839	P1926	K2034	D2096	D2178
PRO	K1496	Y1610	N1673	L1757	V1843	P1927	F2035	L2097	Y2179
GLN	L1502	G1611	V1674	G1758	R1944	S1928	R2036	D2098	K2180
THR	L1502	R1612	V1675	A1759	R1945	F1930	R2037	D2099	T2181
GLY	L1508	R1613	L1676	P1760	M1946	K1931	K2038	S2100	L2182
ALA	V1508	R1614		A1761	T1852	Q1934	E2039	S2101	D2183
PRO	Y1509	R1615		N1762	T1853	Q1940	L2040	K2102	K2185
VAL	G1615	I1616		K1764	E1853	M1940	L2041	R2103	L2186
PRO	I1682	P1617		K1765	F1856	M1941	D2042	K2106	K2187
LEU	E1513	R1618		L1766	L1860	Q1944	R2044	G2107	G2188
ARG	R1516	L1621		G1767	L1861	L1945	R2046	V2108	L2189
ALA	Q1517	A1622		E1768	F1862	P1946	L2047	L2109	L2190
LEU	Q1526	A1623		I1769	D1863	P1946	ASP	S2110	L2191
ASN	F1526	N1624		Y1771	K1864	A1951	ASP	K2111	E2192
ASN	V1530	T1629		L1777	G1865	G1955	LYS	E2112	F2194
VAL	K1531	M1631		G1778	F1866	G1955	TYR	W2115	Q2195
SER	D1535	A1632		I1779	F1867	R1961	ARG	T2116	ASP
GLY	F1536	E1633		T1780	E1868	R1961	GLU	E2117	LEU
VAL	I1543	E1634		Q1781	T1869	F1964	LEU	A2118	ALA
LYS	E1544	H1635		I1782	L1870	L1968	ARG	R2119	L2189
THR		V1636		M1783	S1871	K1969	SER	R2120	LYS
GLU	V1553	P1637		M1786	A1874	K1969	GLN	R2125	ILE
TYR	E1556	L1638		G1787	W1873	Y1981	SER	R2126	ARG
THR	P1557	F1639		W1788	A1874	I1985	ASN	R2127	ASP
GLU	I1562	Q1640		S1789	V1877	I1985	LYS	R2128	HIS
VAL	T1562	V1641		H1790		I1985	SER	R2129	ASP
LYS	M1564	A1642		L1791		Y1988	LEU	L2130	ASN
ASN	V1565	N1644		T1792	R1881	Y1988	ALA	E2131	ASP
ALA	A1646	D1645		L1797	A1882	P1990	PRO	E2132	ALA
GLY	A1647	A1646			L1883	P1991	GLU	E2133	ILE
GLU	F1647	A1647			L1884	P1991	VAL		ASP
TRP	K1568	M1648			I1887	T1992	HIS	T2136	LEU
VAL	I1569	P1649			P1888	S1999	GLN	L2139	SER
PHE	T1570	D1650			P1888	W2000	ILE	S2140	GLU
LYS	V1571	K1651			M1807	V2001	SER	R2141	VAL
SER	G1579	G1652			V1810	L1902	LYS	Q2142	LYS
LEU	R1580	Q1654			P1811	T1903	GLN	V2143	LYS
GLY	Q1581	Y1655			A1812	P1904	LEU	G2144	LYS
LYS	F1582	L1656			K1813	A1905	ALA	A2146	LYS
PRO	V1583	Y1657			R1814	D1907	ASP	S2147	ASP
GLY	V1584	L1658			N1815	P1907	ALA	R2148	LYS
SER	V1585	T1659			I1820	P1910	ARG	L2149	LYS
LYS	A1586	E1661			N1911	S1912	GLU	R2150	LYS
HIS	N1587	G1662			S1912	A2016	ARG	K2151	GLY
L1480	K1592	M1663			A1913	D2017	E2081	L2082	LYS
R1481	I1593	T1665			T1915	V2018	L2083	L2083	LYS
P1482	Q1599	L1686			Q1918	N2019	P2084	L2084	LYS
I1483	E1602	K1687			E1919	A2020	T2085	L2085	LYS
A1484	P1603	K1688			G1921	A2021	R2086	R2086	LYS
T1485						A2022	G2087	G2087	LYS
P1486						V2024	Q2088	Q2088	LYS
Y1487							L2089	L2089	LYS
P1488							V2024	S2090	LYS

• Molecule 1: ACETYL-COENZYME A CARBOXYLASE



ILE	VAL	E1602
LYS	LYS	F1603
ASP	GLU	K1606
PRO	V1492	V1492
GLN	L1493	V1493
THR	Q1494	V1494
GLY	T1505	Y1610
ALA	T1505	A1611
PRO	V1508	R1612
VAL	I1616	I1616
LEU	R1516	P1617
ARG	S1519	R1618
ALA	S1520	I1619
LEU	S1521	A1623
ILE	S1522	G1624
ASN	Q1523	M1625
ASN	K1524	P1629
VAL	S1527	A1632
SER	G1530	E1633
GLY	V1530	E1634
TYR	T1533	I1635
ILE	F1537	V1636
VAL	L1542	P1637
THR	D1545	L1638
GLU	E1546	F1639
VAL	M1547	Q1640
LYS	G1548	V1641
ASN	A1549	A1642
ALA	L1550	V1643
LYS	A1551	N1644
GLY	E1552	A1646
GLU	N1553	A1647
TRP	E1556	N1648
VAL	P1557	P1649
PHE	K1568	K1651
LYS	I1569	G1652
LEU	T1570	F1653
LYS	V1571	Q1654
SER	E1575	L1656
LEU	R1580	Y1657
GLY	Q1581	L1658
LYS	V1585	T1659
ARG	A1586	S1660
PRO	M1587	E1661
ILE	P1598	
ALA	S1674	
THR	V1675	
PRO		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.44 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.226 , 0.262 0.225 , 0.260	Depositor DCC
$R_{free}$ test set	11315 reflections (11.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<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:  
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(°)	Ideal(°)
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:H	1:B:1735:ILE:HD13	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%)	5	11
1	B	680/805 (84%)	602 (88%)	64 (9%)	14 (2%)	8	21
1	C	668/805 (83%)	582 (87%)	66 (10%)	20 (3%)	5	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2028/2415 (84%)	1773 (87%)	200 (10%)	55 (3%)	6	15

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 ⓘ

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%)	15	33
1	B	579/668 (87%)	528 (91%)	51 (9%)	12	27
1	C	568/668 (85%)	513 (90%)	55 (10%)	9	22
All	All	1726/2004 (86%)	1575 (91%)	151 (9%)	12	27

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

Mol	Chain	Res	Type
1	B	1791	LEU
1	B	2100	SER
1	C	1960	GLN
1	B	1797	LEU
1	B	1924	TRP

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

Mol	Chain	Res	Type
1	B	1624	ASN
1	B	1790	HIS

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Mol	Chain	Res	Type
1	C	1941	ASN
1	B	1752	GLN
1	B	1837	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 ⓘ

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	1.53	2 (22%)	7,15,15	1.27	1 (14%)

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	-	-	0/0/0/0	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	C4-N9	2.35	1.39	1.34
2	C	3196	ADE	C2-N3	3.02	1.37	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3196	ADE	N3-C2-N1	-2.39	126.78	128.86

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, 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	667/805 (82%)	-0.05	28 (4%)	37 35	20, 36, 74, 88	0
1	B	667/805 (82%)	0.05	46 (6%)	18 16	21, 38, 77, 94	0
1	C	655/805 (81%)	0.02	36 (5%)	26 24	23, 39, 77, 92	0
All	All	1989/2415 (82%)	0.00	110 (5%)	26 24	20, 38, 76, 94	0

The worst 5 of 110 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 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( $\text{\AA}^2$ )	Q<0.9
2	ADE	C	3196	10/10	0.69	0.36	5.24	86,87,87,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.