wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:03 AM GMT

PDB ID	:	3H0J
Title	:	Crystal structure of the carboxyltransferase domain of acetyl-coenzyme A carboxylase in complex with compound 2
Authors	:	Zhang, H.; Tong, L.
Deposited on	:	2009-04-09
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

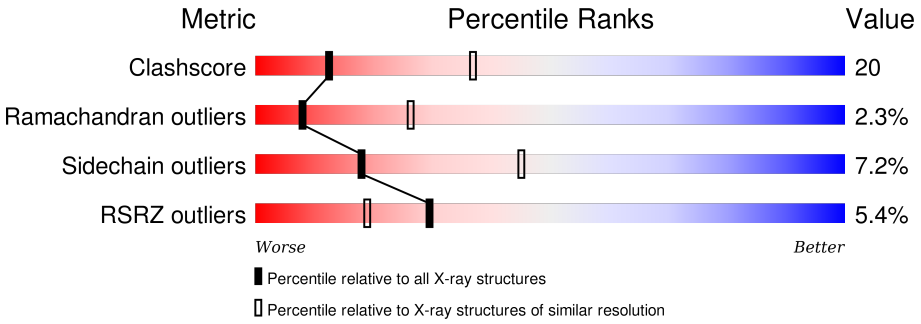
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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 <=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	769	4% 57% 28% • 11%
1	B	769	5% 50% 33% • 12%
1	C	769	5% 55% 27% • 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16200 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-CoA carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	681	Total	C	N	O	S	0	0	0
			5424	3459	930	1016	19			
1	B	675	Total	C	N	O	S	0	0	0
			5376	3427	923	1007	19			
1	C	665	Total	C	N	O	S	0	0	0
			5298	3374	912	993	19			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1473	MET	-	EXPRESSION TAG	UNP Q00955
A	1474	ALA	-	EXPRESSION TAG	UNP Q00955
A	1475	SER	-	EXPRESSION TAG	UNP Q00955
A	2234	LEU	-	EXPRESSION TAG	UNP Q00955
A	2235	GLU	-	EXPRESSION TAG	UNP Q00955
A	2236	HIS	-	EXPRESSION TAG	UNP Q00955
A	2237	HIS	-	EXPRESSION TAG	UNP Q00955
A	2238	HIS	-	EXPRESSION TAG	UNP Q00955
A	2239	HIS	-	EXPRESSION TAG	UNP Q00955
A	2240	HIS	-	EXPRESSION TAG	UNP Q00955
A	2241	HIS	-	EXPRESSION TAG	UNP Q00955
B	1473	MET	-	EXPRESSION TAG	UNP Q00955
B	1474	ALA	-	EXPRESSION TAG	UNP Q00955
B	1475	SER	-	EXPRESSION TAG	UNP Q00955
B	2234	LEU	-	EXPRESSION TAG	UNP Q00955
B	2235	GLU	-	EXPRESSION TAG	UNP Q00955
B	2236	HIS	-	EXPRESSION TAG	UNP Q00955
B	2237	HIS	-	EXPRESSION TAG	UNP Q00955
B	2238	HIS	-	EXPRESSION TAG	UNP Q00955
B	2239	HIS	-	EXPRESSION TAG	UNP Q00955
B	2240	HIS	-	EXPRESSION TAG	UNP Q00955
B	2241	HIS	-	EXPRESSION TAG	UNP Q00955
C	1473	MET	-	EXPRESSION TAG	UNP Q00955

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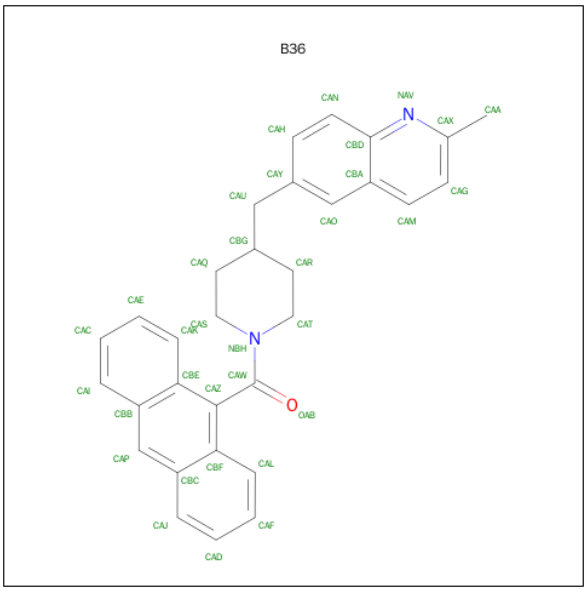
Chain	Residue	Modelled	Actual	Comment	Reference
C	1474	ALA	-	EXPRESSION TAG	UNP Q00955
C	1475	SER	-	EXPRESSION TAG	UNP Q00955
C	2234	LEU	-	EXPRESSION TAG	UNP Q00955
C	2235	GLU	-	EXPRESSION TAG	UNP Q00955
C	2236	HIS	-	EXPRESSION TAG	UNP Q00955
C	2237	HIS	-	EXPRESSION TAG	UNP Q00955
C	2238	HIS	-	EXPRESSION TAG	UNP Q00955
C	2239	HIS	-	EXPRESSION TAG	UNP Q00955
C	2240	HIS	-	EXPRESSION TAG	UNP Q00955
C	2241	HIS	-	EXPRESSION TAG	UNP Q00955

- Molecule 2 is 6-{[1-(ANTHRACEN-9-YLCARBONYL)PIPERIDIN-4-YL]METHYL}-2-METHYLQUINOLINE (three-letter code: B36) (formula: $C_{31}H_{28}N_2O$).



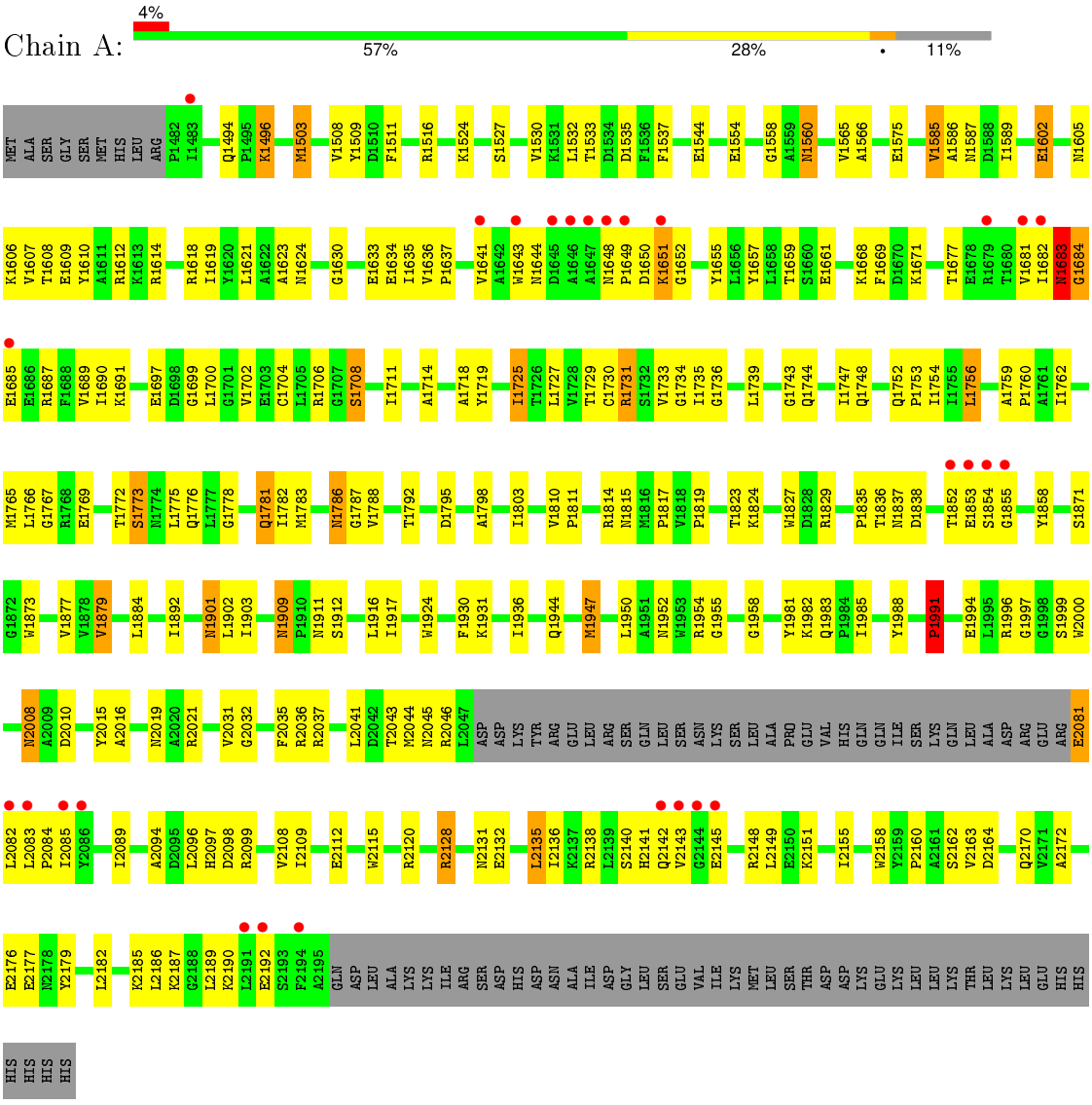
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	31	2	1		
2	B	1	Total	C	N	O	0	0
			34	31	2	1		
2	C	1	Total	C	N	O	0	0
			34	31	2	1		

3 Residue-property plots (i)

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.

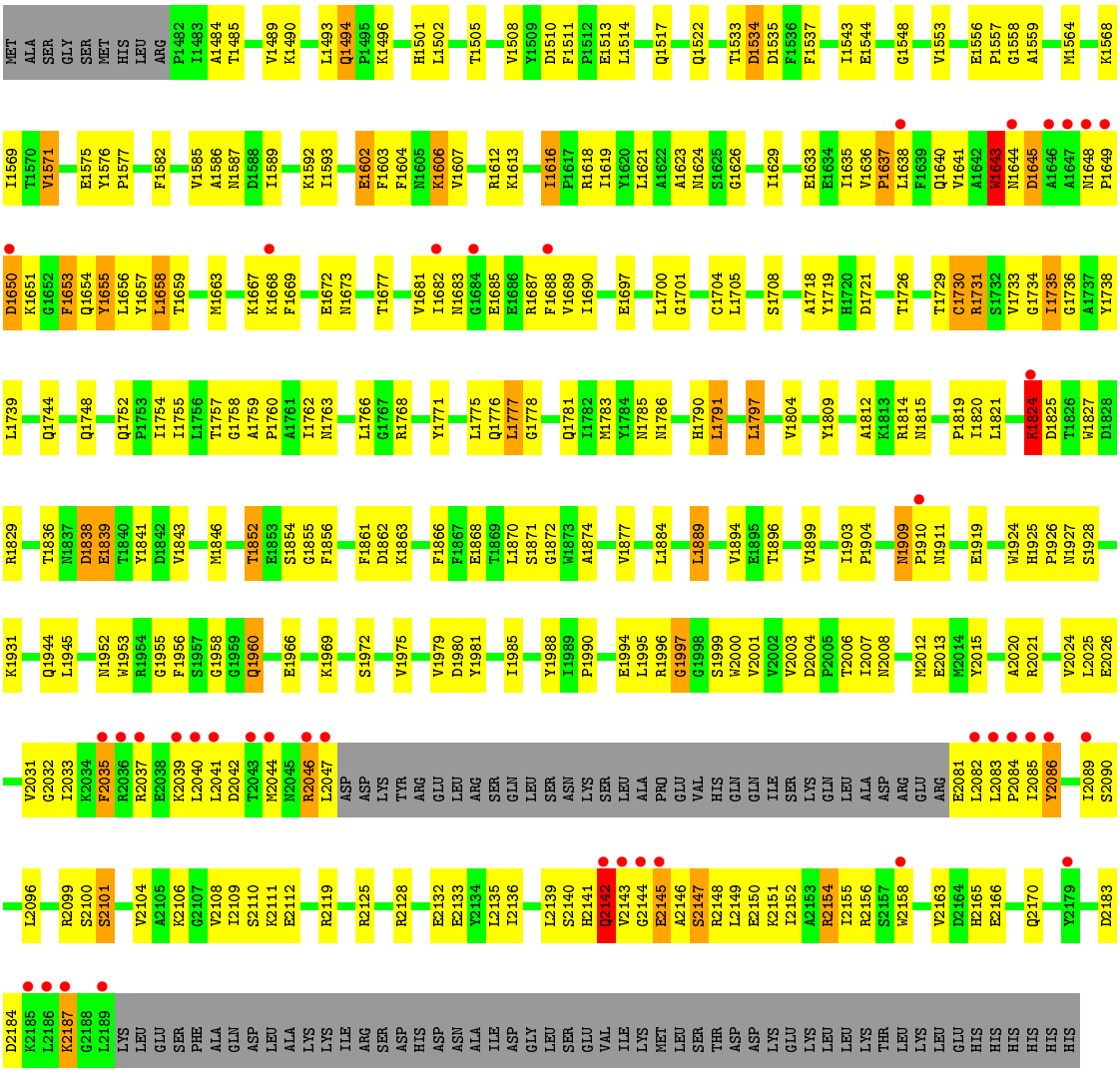
- Molecule 1: Acetyl-CoA carboxylase

Chain A:



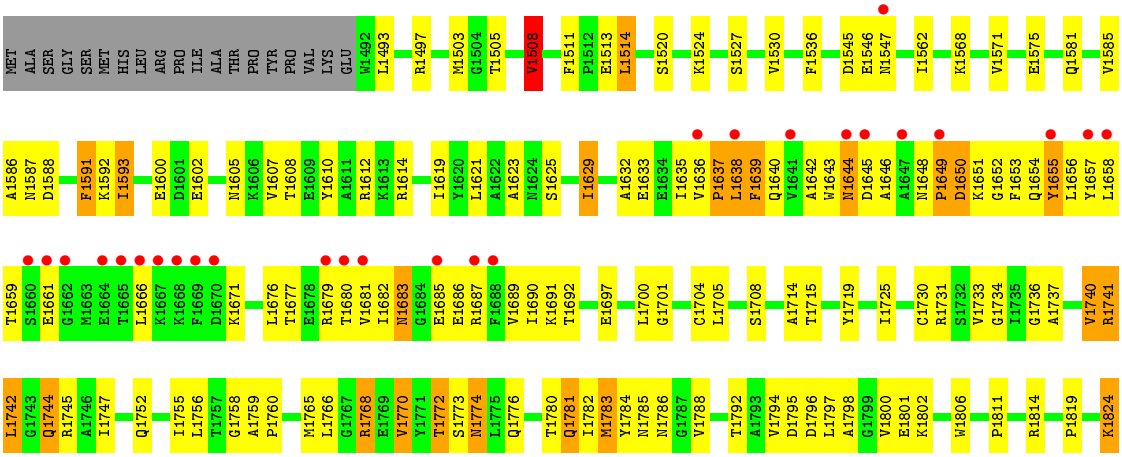
- Molecule 1: Acetyl-CoA carboxylase

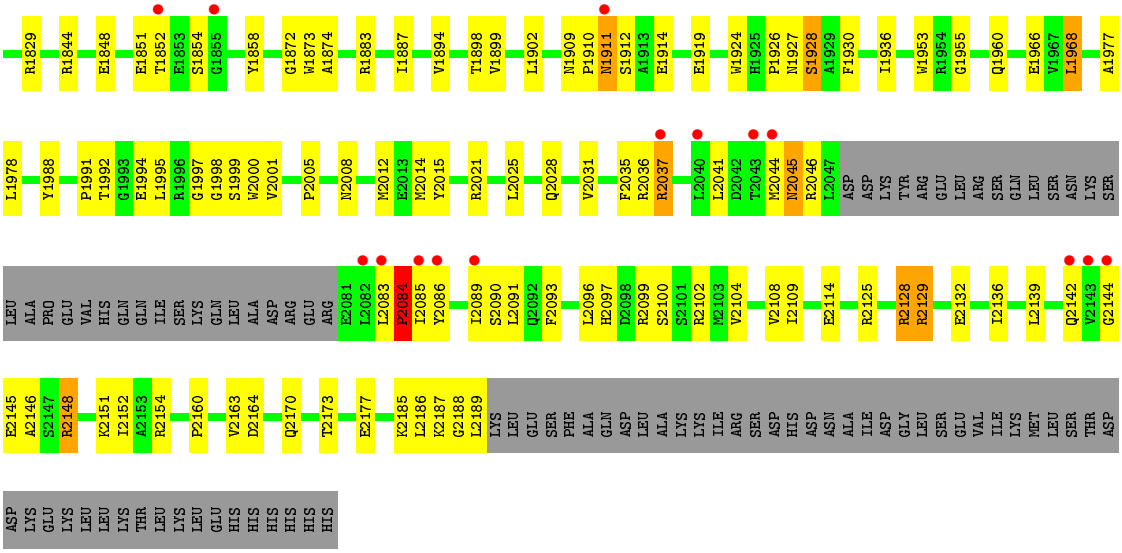
Chain B:



• Molecule 1: Acetyl-CoA carboxylase

Chain C:




R1829 R1844 E1848 E1851 T1852 E1853 S1854 G1855 Y1858 G1872 W1873 A1874 R1883 I1887 V1894 T1898 V1899 L1902 N1909 P1910 N1911 S1912 A1913 E1914 E1919 W1924 H1925 P1926 N1927 S1928 A1929 F1930 I1936 W1953 R1954 G1955 Q1960 E1966 V1967 L1968 A1977
L1978 Y1988 P1991 T1992 G1993 E1994 L1995 R1996 G1997 G1998 S1999 W2000 V2001 P2005 N2008 M2012 E2013 M2014 Y2015 R2021 L2025 Q2028 V2031 F2035 R2036 R2037 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 I2089 S2090 L2091 Q2092 F2093 L2096 H2097 D2098 R2099 S2100 S2101 R2102 M2103 V2104 V2108 I2109 E2114 R2125 R2128 R2129 E2132 I2136 L2139 Q2142 V2143 G2144
E2145 A2146 S2147 R2148 K2151 I2152 A2153 R2154 P2160 V2163 D2164 Q2170 T2173 E2177 K2185 L2186 K2187 G2188 L2189 LYS LEU GLU SER PHE ALA GLN ASP LEU ALA LYS LYS ILE ARG SER ASP HIS ASP ASN ALA ILE ASP GLY LEU SER GLU VAL ILE LYS MET LEU SER THR ASP
ASP LYS GLU LYS LEU LEU LYS THR LEU LYS LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	246.74Å 122.86Å 145.88Å 90.00° 93.92° 90.00°	Depositor
Resolution (Å)	51.25 – 2.80 51.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (51.25-2.80) 99.3 (51.25-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.13 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.257 0.225 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 106688 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16200	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B36

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	0.38	0/5546	0.66	0/7514
1	B	0.36	0/5497	0.65	1/7449 (0.0%)
1	C	0.36	0/5415	0.64	0/7335
All	All	0.37	0/16458	0.65	1/22298 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1791	LEU	CA-CB-CG	5.60	128.17	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5424	0	5365	211	0
1	B	5376	0	5316	222	0
1	C	5298	0	5234	220	0
2	A	34	0	28	1	0
2	B	34	0	28	2	0
2	C	34	0	28	1	0
All	All	16200	0	15999	628	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 20.

The worst 5 of 628 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:1494:GLN:HA	1:A:1496:LYS:HE3	1.39	0.99
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.43	0.99
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.04	0.97
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.61	0.97
1:C:1772:THR:H	1:C:1776:GLN:HE22	1.00	0.95

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	677/769 (88%)	608 (90%)	58 (9%)	11 (2%)	12 38
1	B	671/769 (87%)	589 (88%)	63 (9%)	19 (3%)	6 21
1	C	661/769 (86%)	585 (88%)	60 (9%)	16 (2%)	7 25
All	All	2009/2307 (87%)	1782 (89%)	181 (9%)	46 (2%)	8 26

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1683	ASN
1	B	1643	TRP
1	B	1731	ARG
1	B	1839	GLU
1	B	2142	GLN

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	577/658 (88%)	543 (94%)	34 (6%)	24 57
1	B	572/658 (87%)	522 (91%)	50 (9%)	13 35
1	C	563/658 (86%)	523 (93%)	40 (7%)	18 46
All	All	1712/1974 (87%)	1588 (93%)	124 (7%)	18 45

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1735	ILE
1	B	2001	VAL
1	C	2028	GLN
1	B	1777	LEU
1	B	1852	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1748	GLN
1	B	1944	GLN
1	C	1941	ASN
1	B	1752	GLN
1	B	1909	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	B36	A	1	-	39,39,39	2.76	23 (58%)	56,56,56	1.43	8 (14%)
2	B36	B	1	-	39,39,39	3.69	31 (79%)	56,56,56	1.26	4 (7%)
2	B36	C	1	-	39,39,39	3.49	27 (69%)	56,56,56	1.31	6 (10%)

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	B36	A	1	-	-	0/12/22/22	0/6/6/6
2	B36	B	1	-	-	0/12/22/22	0/6/6/6
2	B36	C	1	-	-	0/12/22/22	0/6/6/6

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	B36	CAL-CBF	2.04	1.46	1.42
2	B	1	B36	CAU-CBG	2.08	1.59	1.53
2	C	1	B36	CAQ-CBG	2.20	1.58	1.52
2	A	1	B36	CBD-NAV	2.21	1.41	1.37
2	A	1	B36	CAF-CAD	2.24	1.43	1.38

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	B36	OAB-CAW-CAZ	-2.96	118.70	121.64
2	B	1	B36	CBA-CBD-NAV	-2.92	117.21	122.25
2	A	1	B36	CBF-CAZ-CBE	-2.82	117.27	120.93
2	A	1	B36	CBA-CBD-NAV	-2.73	117.55	122.25
2	A	1	B36	CAI-CBB-CAP	-2.40	117.92	121.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	B36	1	0
2	B	1	B36	2	0
2	C	1	B36	1	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

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^{th} 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	681/769 (88%)	-0.03	28 (4%)	41	29	24, 43, 89, 107	0
1	B	675/769 (87%)	0.08	39 (5%)	26	16	22, 46, 102, 119	0
1	C	665/769 (86%)	0.10	42 (6%)	23	14	23, 46, 111, 132	0
All	All	2021/2307 (87%)	0.05	109 (5%)	29	19	22, 45, 99, 132	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2037	ARG	5.5
1	C	2082	LEU	5.5
1	B	2082	LEU	5.4
1	B	2143	VAL	5.3
1	B	2086	TYR	4.9

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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^{th} 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^2)	Q<0.9
2	B36	A	1	34/34	0.90	0.25	1.63	65,70,74,74	0
2	B36	C	1	34/34	0.93	0.24	1.50	59,61,63,64	0
2	B36	B	1	34/34	0.89	0.23	0.96	63,68,71,72	0

6.5 Other polymers (i)

There are no such residues in this entry.