



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 12:58 am BST

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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
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)	:	2.11

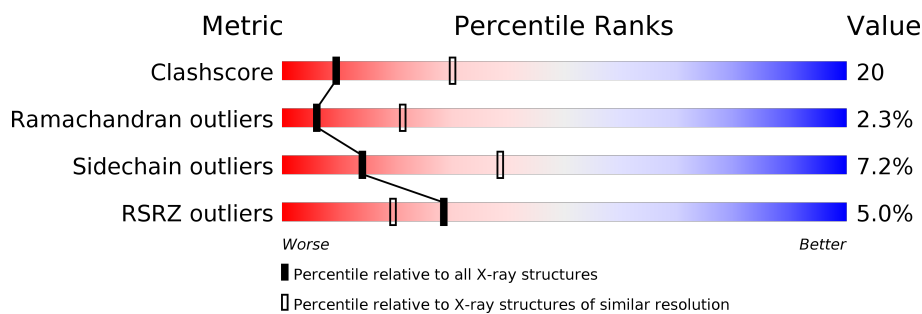
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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 $\leq 5\%$. 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	769	<div> <div>4%</div> <div>57%</div> <div>28%</div> <div>•</div> <div>11%</div> </div>
1	B	769	<div> <div>5%</div> <div>50%</div> <div>33%</div> <div>•</div> <div>12%</div> </div>
1	C	769	<div> <div>5%</div> <div>55%</div> <div>27%</div> <div>•</div> <div>14%</div> </div>

2 Entry composition

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:

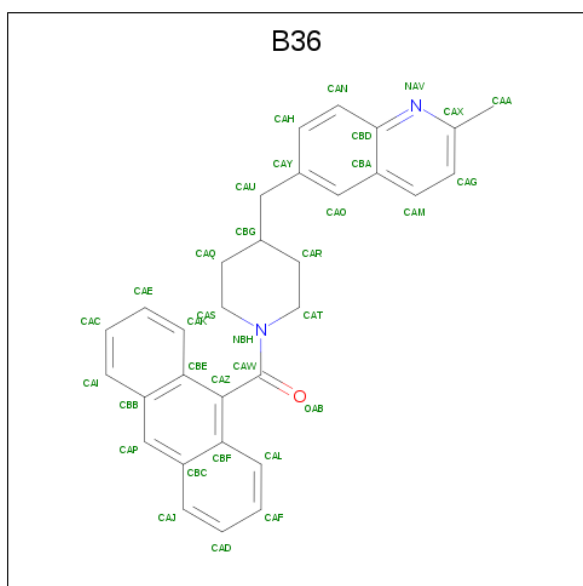
Chain	Residue	Modelled	Actual	Comment	Reference
A	1473	MET	-	EXPRESSION TAG	UNP Q00955
A	1474	ALA	-	EXPRESSION TAG	UNP Q00955
A	1475	SER	-	EXPRESSION TAG	UNP Q00955
A	2234	LEU	-	EXPRESSION TAG	UNP Q00955
A	2235	GLU	-	EXPRESSION TAG	UNP Q00955
A	2236	HIS	-	EXPRESSION TAG	UNP Q00955
A	2237	HIS	-	EXPRESSION 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: C₃₁H₂₈N₂O).



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		



ASP	E2145	LEU	L1978	R1829
LYS	A2146	ALA	Y1988	R1844
GLU	S2147	PRO		
LYS	R2148	GLU		
LEU		VAL	P1991	E1848
LEU	K2151	HIS	T1992	E1851
LYS	T2152	GLN	G1993	T1852
THR	K2153	GLN	E1994	E1853
LEU	K2154	ILE	L1995	S1854
LYS		SER	R1996	G1855
LEU	P2160	LYS	G1997	
GLU		GLN	G1998	Y1858
HIS	V2163	LEU	S1999	
HIS	D2164	ALA	W2000	G1872
HIS		ASP	V2001	W1873
HIS	Q2170	ARG		A1874
HIS	T2173	GLU	P2005	
		ARG		R1883
	E2177	E2081	N2008	I1887
		L2082		V1894
	K2185	L2083	M2012	T1898
	L2186	P2084	E2013	V1899
	K2187	I2085	M2014	L1902
	G2188	Y2086	Y2015	N1909
	L2189			P1910
LYS		I2089	R2021	N1911
LEU		S2090		S1912
GLU		L2091	L2025	A1913
SER		Q2092		E1914
PHE		F2093	Q2028	
ALA			V2031	E1919
GLN		L2096		W1924
ASP		H2097		H1925
LEU		D2098	F2035	P1926
ALA		R2099	R2036	N1927
LYS		S2100	R2037	S1928
LYS		S2101		A1929
LYS		R2102	L2040	F1930
ILE		P2103	L2041	
ARG		V2104	D2042	I1936
SER			T2043	W1953
ASP		V2108	N2044	R1954
HIS		I2109	N2045	G1955
ASP			R2046	Q1960
ASN		E2114	L2047	E1966
ALA			ASP	V1967
ILE		R2125	ASP	L1968
ASP			LYS	
GLY		R2128	TYR	
LEU		R2129	ARG	
SER			GLU	
GLU		E2132	LEU	
VAL			ARG	
ILE		I2136	SER	
LYS		I2139	GLN	
MET			LEU	
LEU		L2139	SER	
SER			ASN	
THR		Q2142	LYS	
ASP		V2143	SER	
		G2144		

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.257 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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(°)	Ideal(°)
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 [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	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:A:1772:THR:H	1:A:1776:GLN:NE2	1.61	0.97
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.04	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%)	9	31
1	B	671/769 (87%)	589 (88%)	63 (9%)	19 (3%)	5	17
1	C	661/769 (86%)	585 (88%)	60 (9%)	16 (2%)	6	20
All	All	2009/2307 (87%)	1782 (89%)	181 (9%)	46 (2%)	6	21

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%)	19	49
1	B	572/658 (87%)	522 (91%)	50 (9%)	10	30
1	C	563/658 (86%)	523 (93%)	40 (7%)	14	39
All	All	1712/1974 (87%)	1588 (93%)	124 (7%)	14	38

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	C	1	-	39,39,39	3.51	27 (69%)	56,56,56	1.32	6 (10%)
2	B36	B	1	-	39,39,39	3.72	30 (76%)	56,56,56	1.27	4 (7%)
2	B36	A	1	-	39,39,39	2.78	23 (58%)	56,56,56	1.46	9 (16%)

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	C	1	-	-	4/12/22/22	0/6/6/6
2	B36	B	1	-	-	2/12/22/22	0/6/6/6
2	B36	A	1	-	-	2/12/22/22	0/6/6/6

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	B36	CAZ-CBE	7.14	1.50	1.41
2	C	1	B36	CAZ-CBF	7.13	1.50	1.41
2	A	1	B36	CAZ-CBE	6.50	1.50	1.41
2	B	1	B36	CAZ-CBF	6.11	1.49	1.41
2	C	1	B36	CBA-CBD	6.07	1.51	1.42

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	B36	CAN-CBD-NAV	3.84	124.55	118.69
2	A	1	B36	CBE-CAZ-CAW	3.83	122.87	119.28
2	B	1	B36	CBA-CBD-NAV	-3.40	117.21	122.26
2	C	1	B36	CBE-CAZ-CAW	3.33	122.40	119.28
2	C	1	B36	CAN-CBD-NAV	3.32	123.75	118.69

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

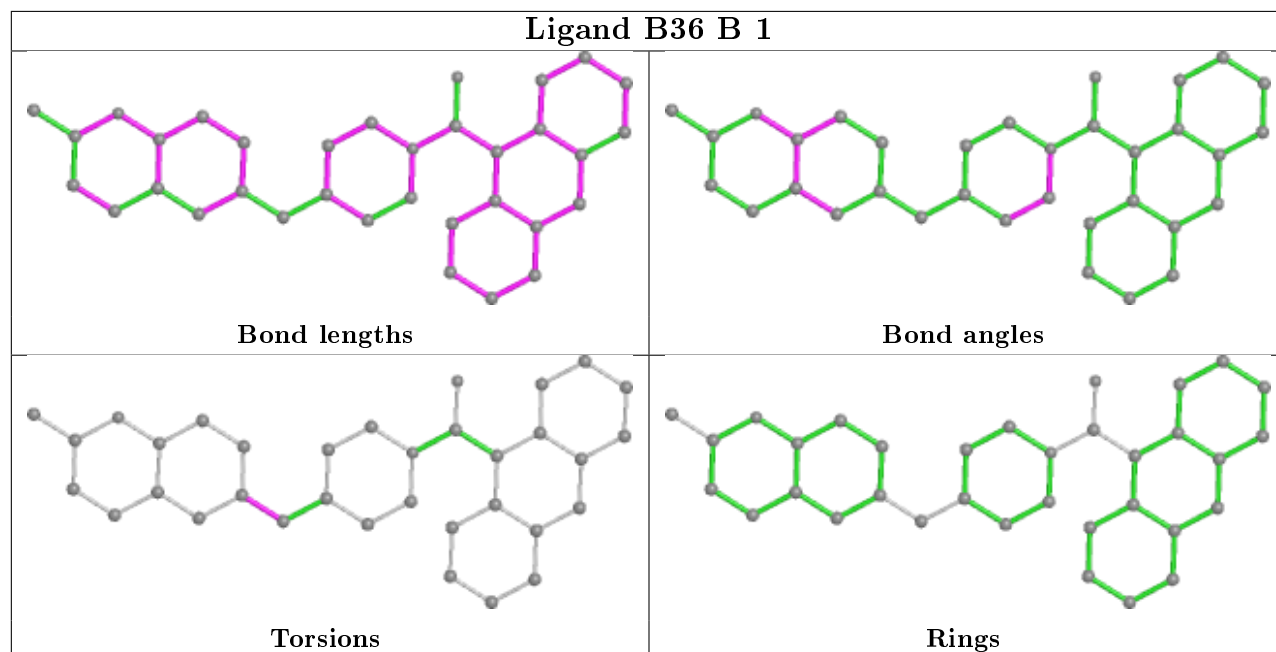
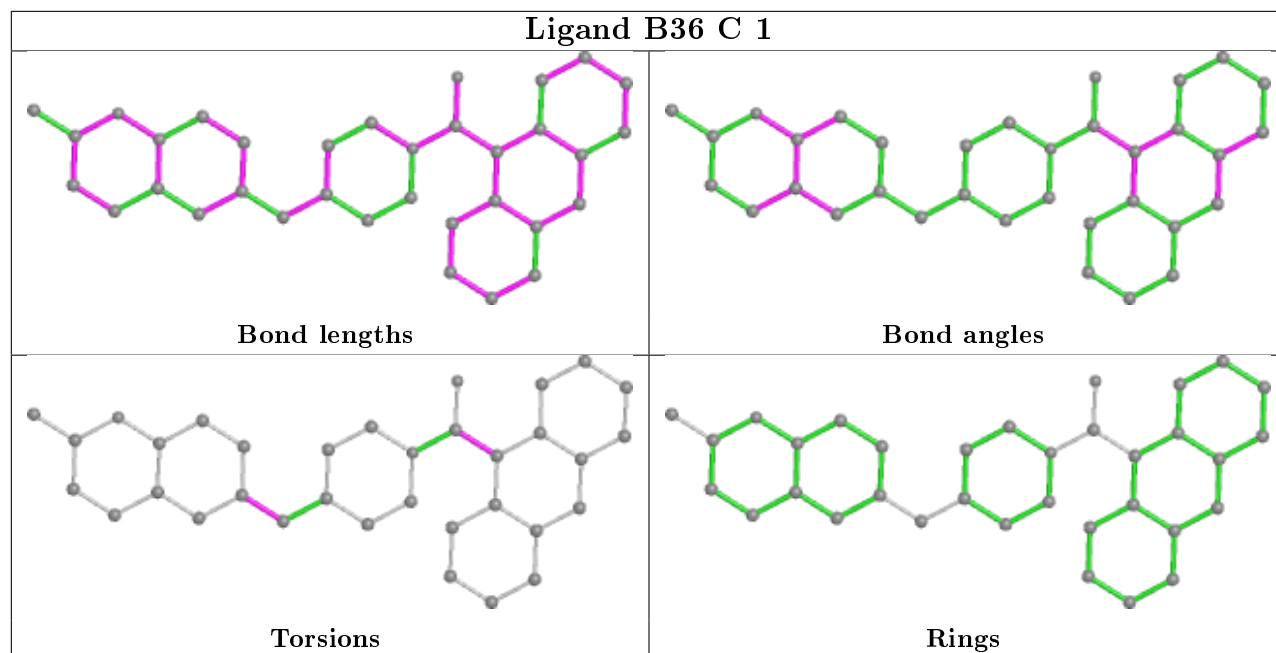
Mol	Chain	Res	Type	Atoms
2	C	1	B36	CBG-CAU-CAY-CAO
2	B	1	B36	CBG-CAU-CAY-CAO
2	B	1	B36	CBG-CAU-CAY-CAH
2	C	1	B36	CBG-CAU-CAY-CAH
2	C	1	B36	NBH-CAW-CAZ-CBE

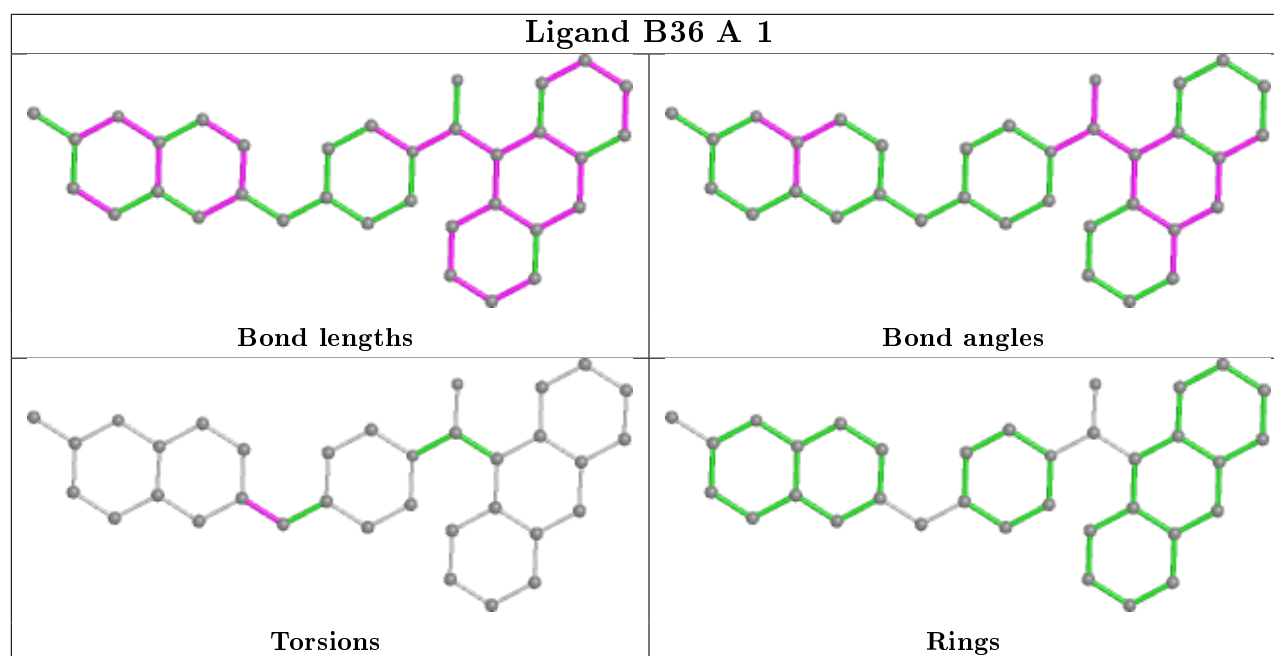
There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	681/769 (88%)	-0.04	27 (3%)	38	28	24, 43, 89, 107	0
1	B	675/769 (87%)	0.07	36 (5%)	26	17	22, 46, 102, 119	0
1	C	665/769 (86%)	0.09	38 (5%)	23	15	23, 46, 111, 132	0
All	All	2021/2307 (87%)	0.04	101 (4%)	28	19	22, 45, 99, 132	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2037	ARG	5.8
1	C	2082	LEU	5.4
1	B	2082	LEU	5.2
1	B	2143	VAL	5.2
1	C	1679	ARG	5.0

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](#)

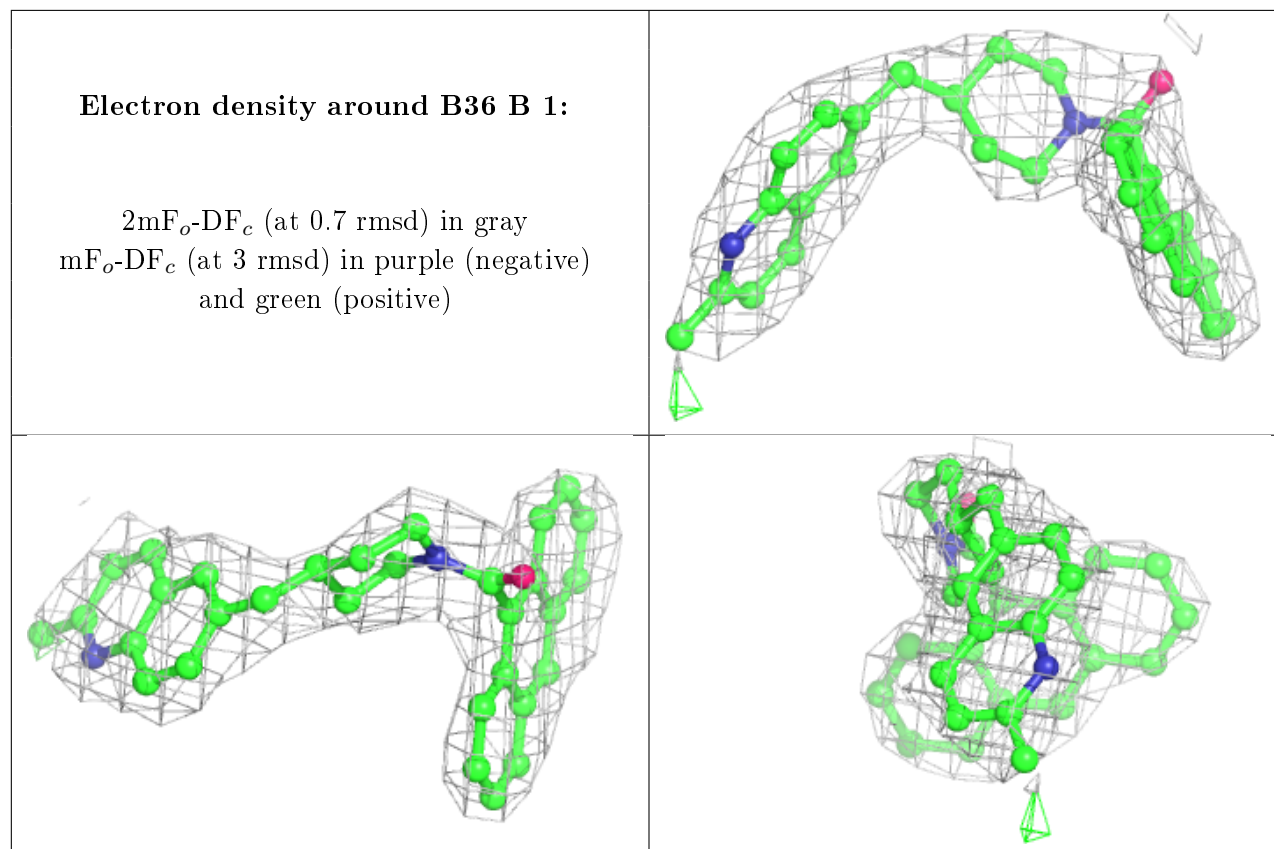
There are no carbohydrates in this entry.

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. 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.

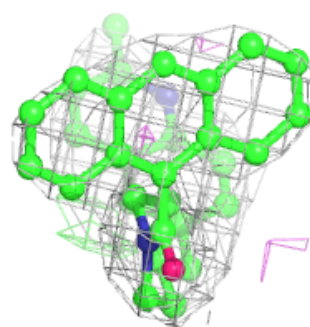
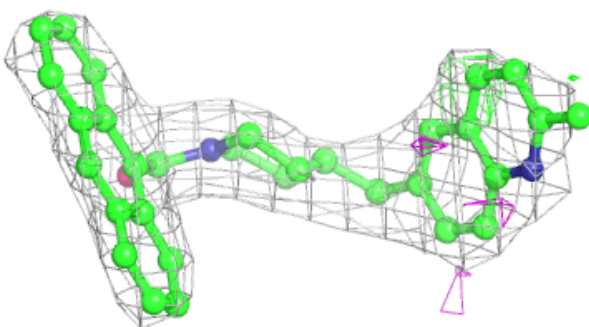
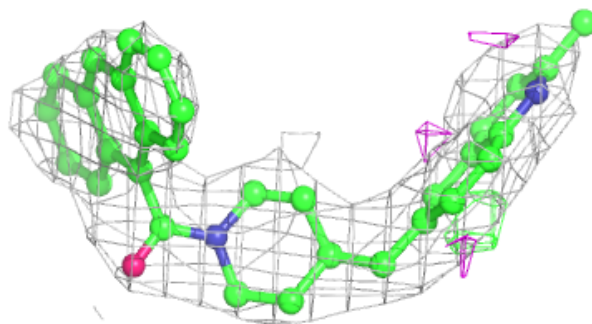
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	B36	B	1	34/34	0.89	0.23	63,68,71,72	0
2	B36	A	1	34/34	0.90	0.25	65,70,74,74	0
2	B36	C	1	34/34	0.93	0.24	59,61,63,64	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

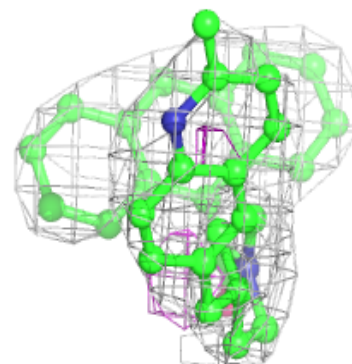
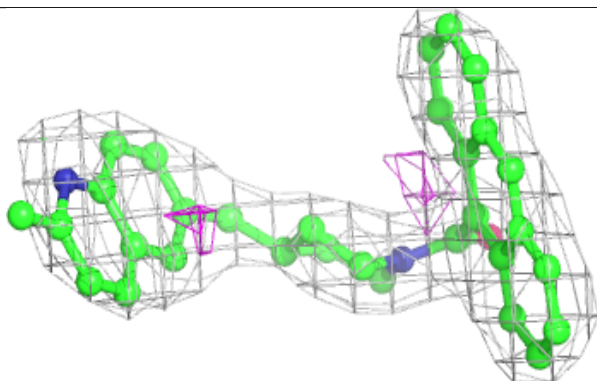
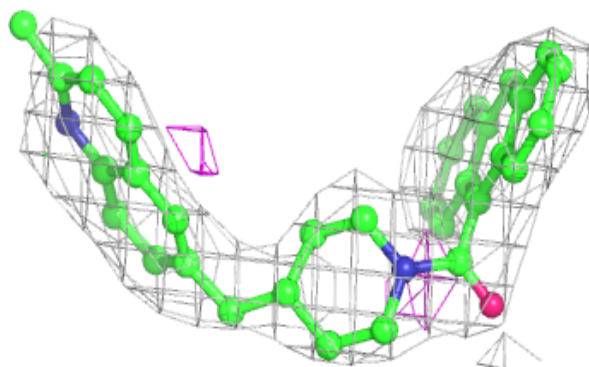


Electron density around B36 A 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around B36 C 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.