



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:52 PM UTC

PDB ID : 1W2X / pdb_00001w2x
Title : Crystal structure of the carboxyltransferase domain of acetyl- coenzyme A
carboxylase in complex with CP-640186
Authors : Zhang, H.; Tweel, B.; Li, J.; Tong, L.
Deposited on : 2004-07-09
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

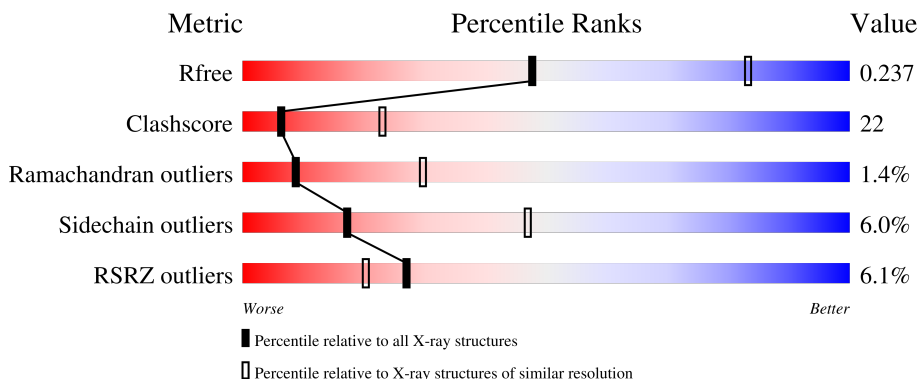
1 Overall quality at a glance

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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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 $\leq 5\%$. 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	758	5% 55% 32% • 10%
1	B	758	7% 50% 35% • 11%
1	C	758	5% 50% 33% 5% 12%

2 Entry composition [i](#)

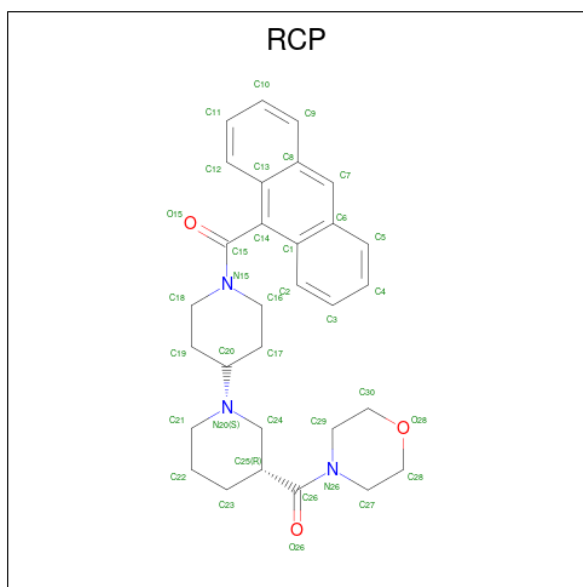
There are 3 unique types of molecules in this entry. The entry contains 16588 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	682	Total	C	N	O	S	0	0	1
			5425	3459	931	1016	19			
1	B	676	Total	C	N	O	S	0	0	1
			5377	3427	924	1007	19			
1	C	666	Total	C	N	O	S	0	0	1
			5299	3374	913	993	19			

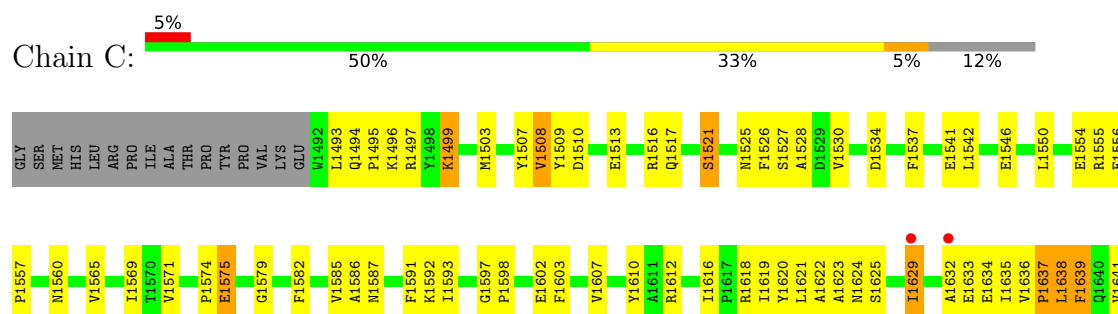
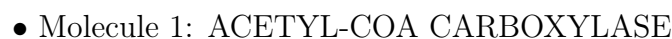
- Molecule 2 is (3R)-1'-(9-ANTHRYLCARBONYL)-3-(MORPHOLIN-4-YLCARBONYL)-1,4'-BIPIPERIDINE (CCD ID: RCP) (formula: C₃₀H₃₅N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	30	3	3		
2	B	1	Total	C	N	O	0	0
			36	30	3	3		
2	C	1	Total	C	N	O	0	0
			36	30	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	147	Total 147	O 147	0	0
3	B	128	Total 128	O 128	0	0
3	C	104	Total 104	O 104	0	0



L2189	L2089	L2025	W1924	L1821	L1727	A1642
K2190	S2090	Q2028	P1926	E1822		W1643
GLU	L2091	G2029		T1823	C1730	N1644
SER	Q2092	M2030	I1936	K1824	R1731	D1645
PHE	F2093	V2031		W1827	S1732	A1647
ALA	S2100	G2032	M1941	D1828	V1733	N1648
GLN	S2101	L2033	Q1944	R1829	G1734	P1649
ASP	L2102	K2034	L1945	F1833	I1735	D1650
LEU	R2102	R2036	P1946		G1736	K1651
ALA	W2103	F2035	M1947		A1737	G1852
LYS	V2104	R2036	M1948			F1853
LYS		R2037			V1740	Q1854
ILE	V2108			R1844	R1741	Y1855
ARG	T2109	L2041	I1949	W1845	L1742	L1656
ASP	S2110	D2042	L1950	M1846		
SER	T2111	T2043		I1847	G1743	Y1657
ASP	T2043	M2044	W1953	E1848	Q1744	L1658
HIS			R1954	G1849	R1745	T1659
ASP	E2114	N2045	G1955	R1850		S1660
ASN	W2115	R2046		E1851	A1746	E1661
ALA		L2047	Q1960	T1852	I1747	G1662
ILE	W2124	ASP	R1961	E1853	Q1752	
ASP		LYS		S1854		L1666
GLY	R2128	ASP	E1966	G1855	I1755	K1667
LEU		TYR	V1967		L1756	K1668
SER	E2132	ARG	L1968	Y1858	T1757	F1669
GLU		GLU			G1758	D1670
VAL	L2135	LEU	L1978	E1868	A1759	K1671
ILE	T2136	ARG	W1979		P1760	E1672
LYS	R2137	SER	D1980	S1871	K1764	
MET	R2138	GLN	Y1981	V1879		L1676
LEU		LEU	K1982			T1677
SER	H2141	SER	Q1983	R1883	V1770	E1678
THR	Q2142	ASN	P1984		Y1771	R1679
ASP	T2143	LYS	I1985		T1772	T1680
ASP	G2144	SER	I1986	T1887	S1773	V1681
LYS	E2145	LEU	I1987	P1888	N1774	I1682
GLU	A2146	ALA		L1889	L1775	G1683
LYS		PRO	P1990	G1890	Q1776	E1684
LEU		GLU	P1991			E1685
LEU	T2151	VAL	T1992	V1894	T1780	E1686
LEU	T2152	GLN	G1993	E1895	Q1781	R1687
LYS	A2153	HIS		T1896	I1782	F1688
THR	R2154	GLN	E1994	R1897	M1783	V1689
LEU	T2155	GLN	L1995	T1898	Y1784	I1690
LYS	R2156	ILE	R1996		N1785	
	S2157	SER	G1997			
		LYS	G1998	L1902	N1786	
	P2160	GLN	S1999	I1903	G1787	I1693
		LEU	W2000	P1904	V1788	
	V2163	ALA	V2001	A1905		G1701
	D2164	ASP		D1906	T1792	C1704
		ARG	D2004	P1907		L1705
	R2169	GLU	P2005	A1908	K1802	
	Q2170	ARG	T2006	N1909		S1708
		E2061		P1910	M1807	G1709
	K2180	L2082	M2014	N1911		
		L2083	D2017	S1912	R1814	A1712
	K2185	P2084			N1815	
	L2186			P1920	W1924	Y1719
						H1720

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.59Å 124.60Å 145.60Å 90.00° 93.85° 90.00°	Depositor
Resolution (Å)	29.66 – 2.80 29.66 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.7 (29.66-2.80) 89.8 (29.66-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.234 0.199 , 0.237	Depositor DCC
R_{free} test set	10186 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.2	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	0.93	EDS
Total number of atoms	16588	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.46	1/5547 (0.0%)	0.95	22/7516 (0.3%)
1	B	0.46	2/5498 (0.0%)	0.96	24/7451 (0.3%)
1	C	0.45	1/5416 (0.0%)	0.92	19/7337 (0.3%)
All	All	0.46	4/16461 (0.0%)	0.94	65/22304 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2012	MET	SD-CE	-5.64	1.65	1.79
1	B	2189	LEU	C-N	-5.55	1.25	1.33
1	A	2195	ALA	C-N	-5.39	1.25	1.33
1	C	2189	LEU	C-N	-5.39	1.25	1.33

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1989	ILE	CA-C-N	7.87	128.49	120.38
1	A	1989	ILE	C-N-CA	7.87	128.49	120.38
1	C	1787	GLY	N-CA-C	-7.79	104.33	114.85
1	B	1494	GLN	CA-C-N	7.77	127.43	119.82
1	B	1494	GLN	C-N-CA	7.77	127.43	119.82

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	5425	0	5365	220	0
1	B	5377	0	5316	249	0
1	C	5299	0	5234	267	0
2	A	36	0	35	4	0
2	B	36	0	35	3	0
2	C	36	0	35	3	0
3	A	147	0	0	4	0
3	B	128	0	0	7	0
3	C	104	0	0	1	0
All	All	16588	0	16020	712	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 22.

The worst 5 of 712 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:1813:LYS:HG2	1:A:1816:MET:HE2	1.33	1.05
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.21	1.05
1:A:1936:ILE:HG12	1:A:1947:MET:HE1	1.39	1.02
1:C:1772:THR:H	1:C:1776:GLN:NE2	1.59	1.01
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.09	1.00

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	678/758 (89%)	618 (91%)	52 (8%)	8 (1%)	10 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	672/758 (89%)	611 (91%)	51 (8%)	10 (2%)	8	28
1	C	662/758 (87%)	588 (89%)	64 (10%)	10 (2%)	8	28
All	All	2012/2274 (88%)	1817 (90%)	167 (8%)	28 (1%)	9	30

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2145	GLU
1	B	2189	LEU
1	C	1644	ASN
1	A	1684	GLY
1	A	1997	GLY

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	577/648 (89%)	550 (95%)	27 (5%)	23	57
1	B	572/648 (88%)	535 (94%)	37 (6%)	15	43
1	C	563/648 (87%)	525 (93%)	38 (7%)	15	42
All	All	1712/1944 (88%)	1610 (94%)	102 (6%)	17	47

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1961	ARG
1	C	1629	ILE
1	C	2102	ARG
1	B	2041	LEU
1	C	1508	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1654	GLN
1	C	1960	GLN
1	C	1748	GLN
1	C	1909	ASN
1	C	2142	GLN

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 oligosaccharides 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	RCP	C	3000	-	41,41,41	0.97	1 (2%)	58,58,58	1.27	7 (12%)
2	RCP	A	3000	-	41,41,41	0.98	1 (2%)	58,58,58	1.25	7 (12%)
2	RCP	B	3000	-	41,41,41	0.97	1 (2%)	58,58,58	1.24	7 (12%)

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	RCP	C	3000	-	-	4/20/48/48	0/6/6/6
2	RCP	A	3000	-	-	0/20/48/48	0/6/6/6
2	RCP	B	3000	-	-	4/20/48/48	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3000	RCP	C14-C15	2.99	1.53	1.50
2	B	3000	RCP	C14-C15	2.92	1.53	1.50
2	A	3000	RCP	C14-C15	2.90	1.53	1.50

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3000	RCP	C27-N26-C29	4.04	120.92	112.68
2	B	3000	RCP	C27-N26-C29	3.74	120.31	112.68
2	A	3000	RCP	C16-N15-C18	3.48	119.78	112.68
2	A	3000	RCP	C27-N26-C29	3.47	119.76	112.68
2	B	3000	RCP	C16-N15-C18	3.37	119.56	112.68

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3000	RCP	O26-C26-N26-C29
2	B	3000	RCP	C25-C26-N26-C29
2	C	3000	RCP	O26-C26-N26-C29
2	C	3000	RCP	C25-C26-N26-C29
2	B	3000	RCP	O26-C26-N26-C27

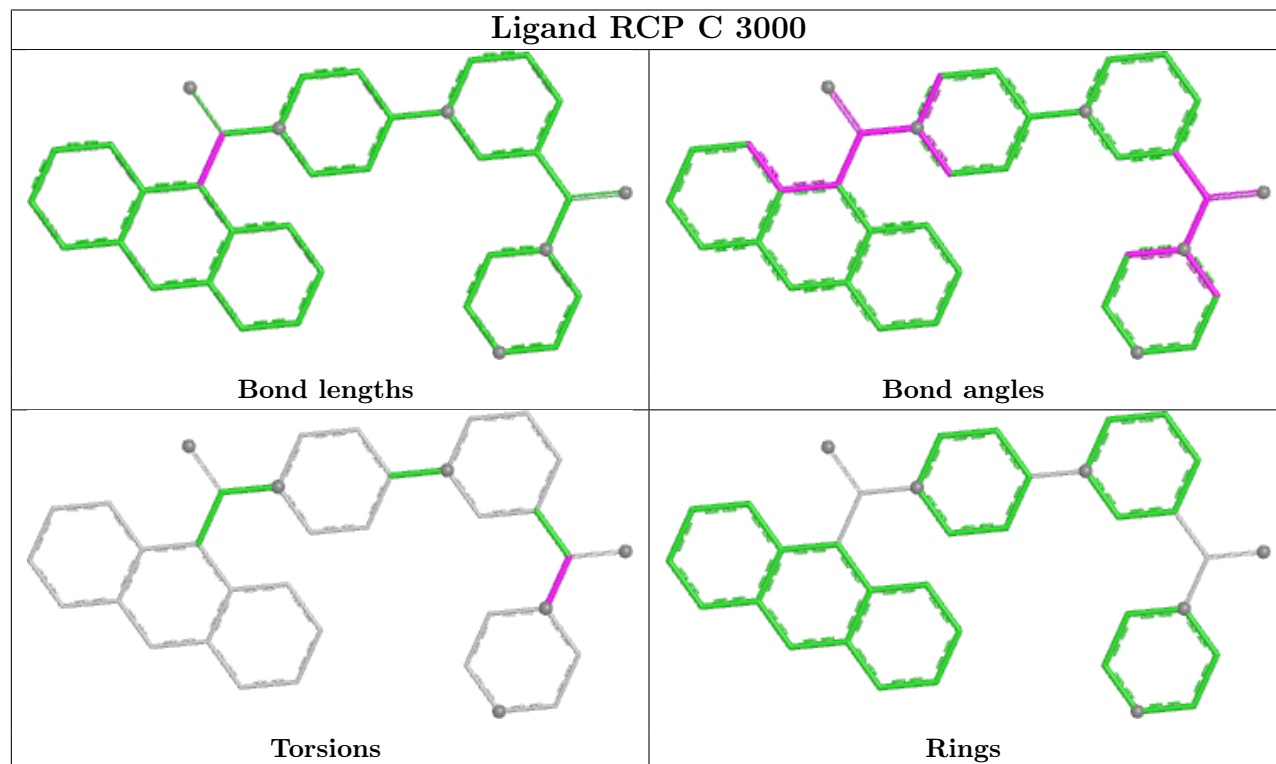
There are no ring outliers.

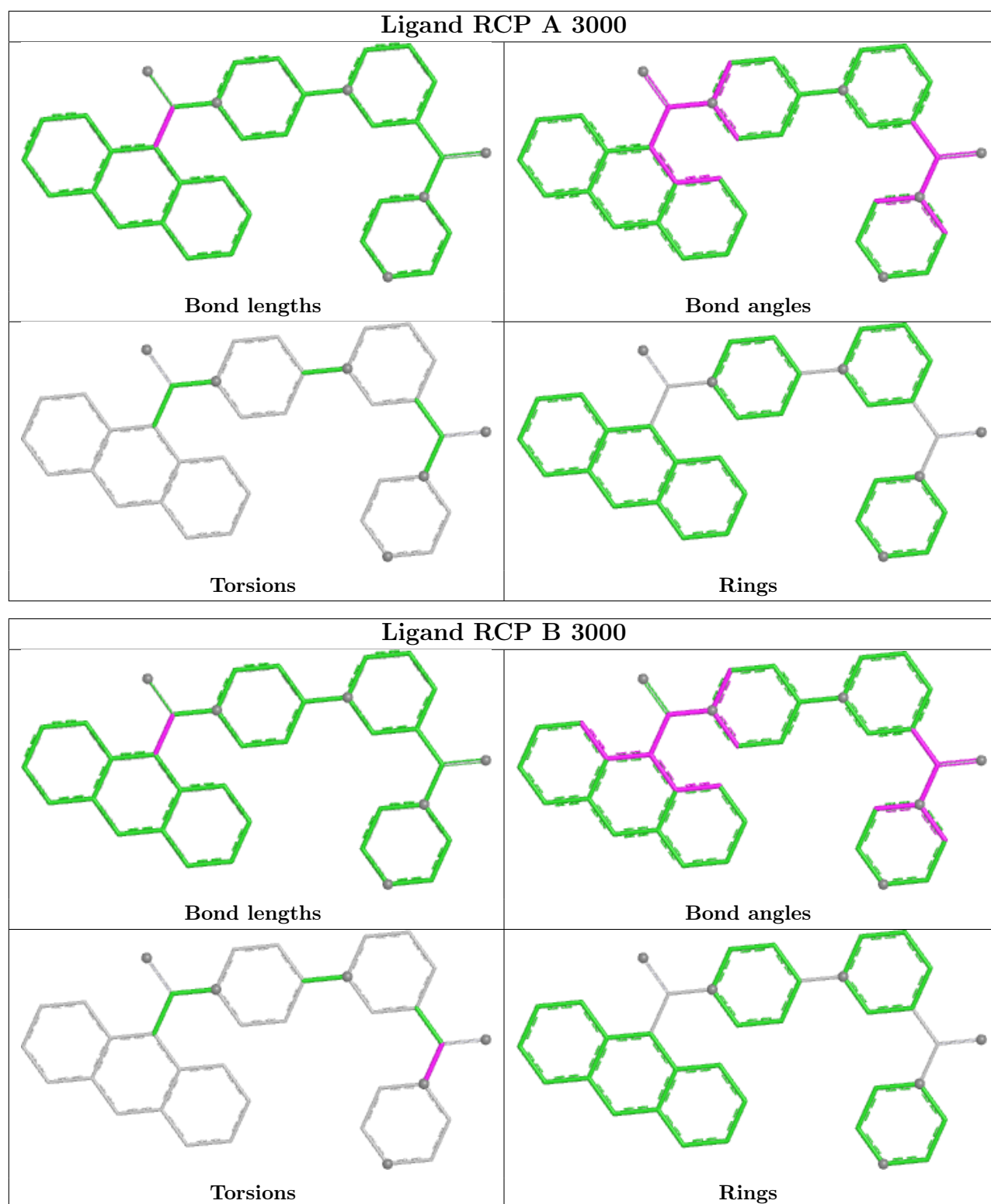
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3000	RCP	3	0
2	A	3000	RCP	4	0
2	B	3000	RCP	3	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 ⓘ

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	682/758 (89%)	0.06	36 (5%)	32	24	22, 47, 98, 99	0
1	B	676/758 (89%)	0.11	50 (7%)	20	15	24, 49, 98, 99	0
1	C	666/758 (87%)	0.06	38 (5%)	29	22	22, 49, 99, 99	0
All	All	2024/2274 (89%)	0.07	124 (6%)	27	20	22, 48, 99, 99	0

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2082	LEU	6.5
1	C	2047	LEU	6.4
1	A	2047	LEU	5.4
1	B	2047	LEU	5.4
1	A	1493	LEU	5.3

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

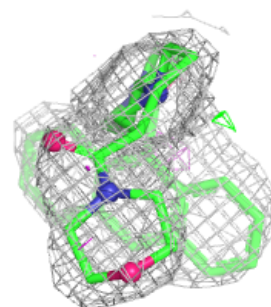
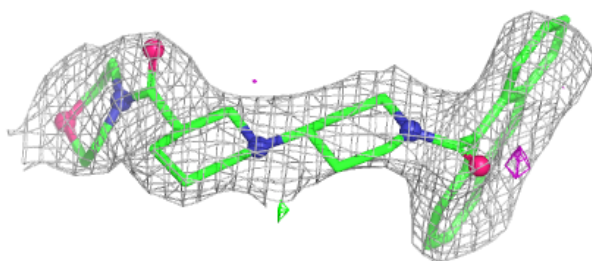
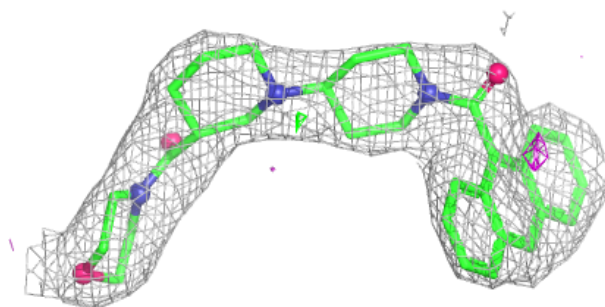
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	RCP	C	3000	36/36	0.92	0.15	73,87,94,95	0
2	RCP	B	3000	36/36	0.94	0.11	58,63,71,71	0
2	RCP	A	3000	36/36	0.95	0.10	60,68,69,70	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.

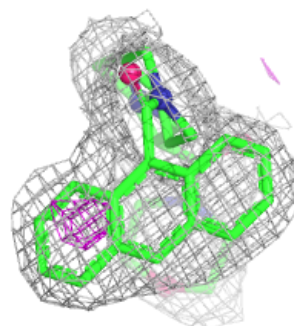
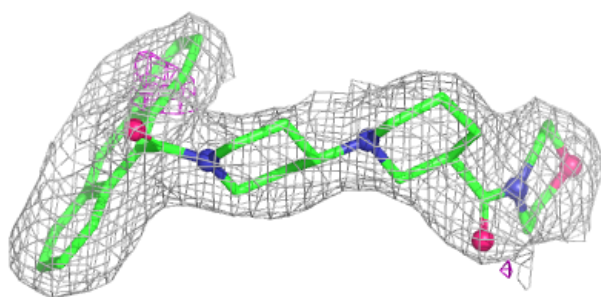
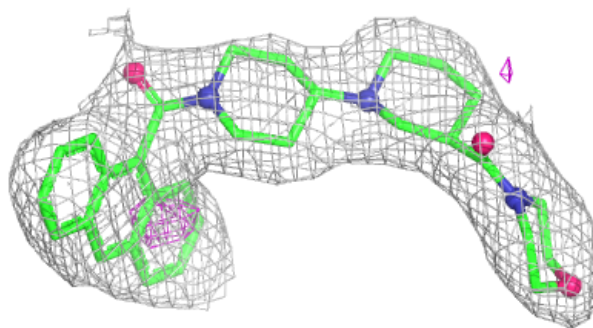
Electron density around RCP C 3000:

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

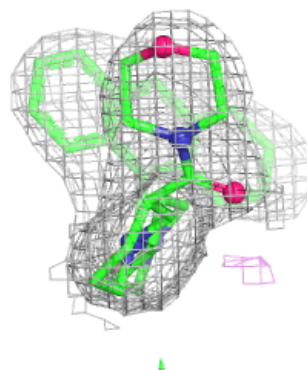
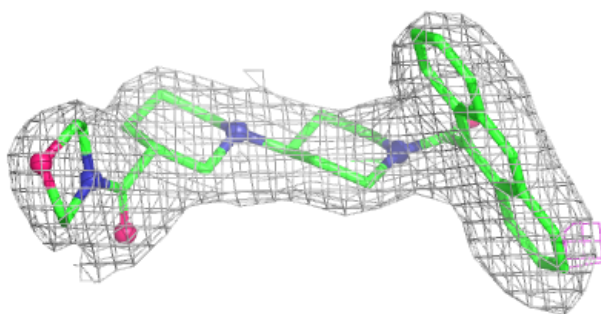
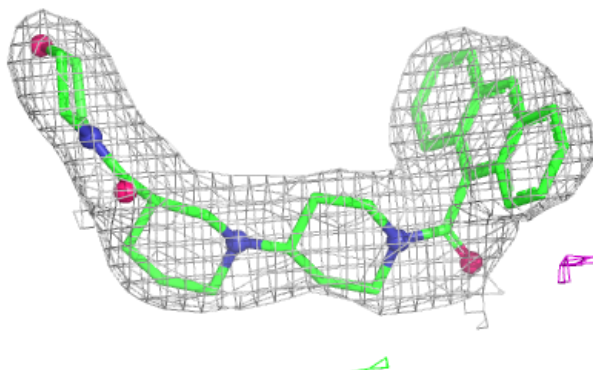


Electron density around RCP B 3000:

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

**Electron density around RCP A 3000:**

$2mF_o-DF_c$ (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.