wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 12:37 pm BST

PDB ID	:	4WYO
Title	:	Crystal structure of human-yeast chimera acetyl coA carboxylase CT domain bound to Compound 1
Authors	:	Vajdos, F.F.
Deposited on	:	2014-11-17
Resolution	:	2.89 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 (i) symbol.

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

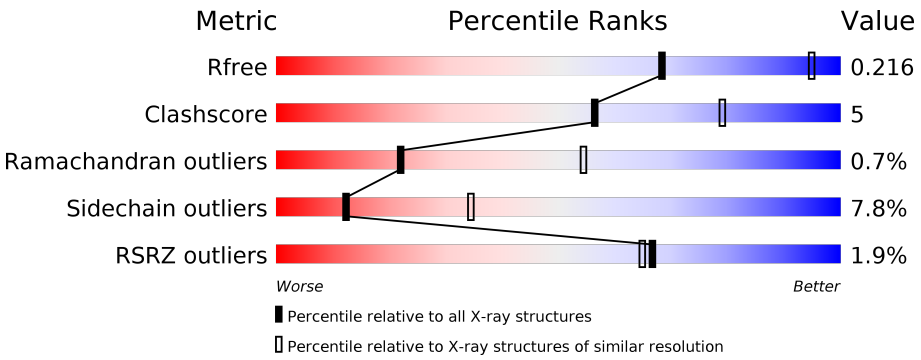
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	B	769	2% 78% 15% • 5%
1	C	769	% 78% 15% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12185 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
			Total	C	N	O	S			
1	B	733	5834	3710	1007	1100	17	0	1	0
1	C	723	5744	3645	992	1089	18	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

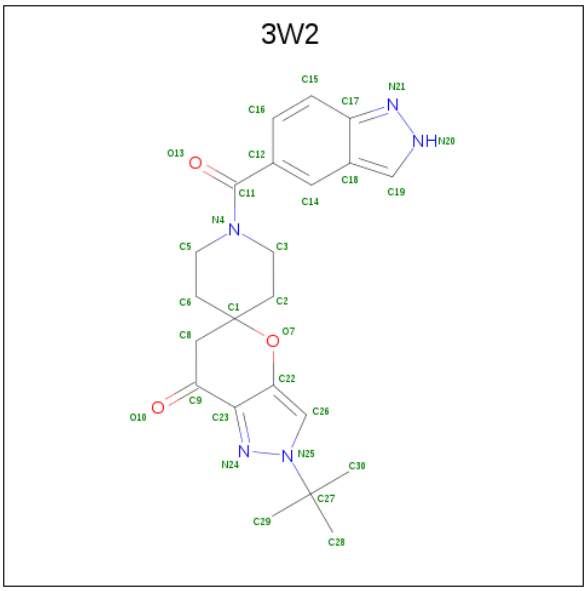
Chain	Residue	Modelled	Actual	Comment	Reference
B	1473	MET	-	initiating methionine	UNP Q00955
B	1474	ALA	-	expression tag	UNP Q00955
B	1475	SER	-	expression tag	UNP Q00955
B	1760	SER	PRO	engineered mutation	UNP Q00955
B	1762	LEU	ILE	engineered mutation	UNP Q00955
B	1765	VAL	MET	engineered mutation	UNP Q00955
B	1919	GLN	GLU	engineered mutation	UNP Q00955
B	1920	ALA	PRO	engineered mutation	UNP Q00955
B	1925	PHE	HIS	engineered mutation	UNP Q00955
B	2028	GLU	GLN	engineered mutation	UNP Q00955
B	2030	THR	MET	engineered mutation	UNP Q00955
B	2032	GLU	GLY	engineered mutation	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	-	initiating methionine	UNP Q00955
C	1474	ALA	-	expression tag	UNP Q00955
C	1475	SER	-	expression tag	UNP Q00955
C	1760	SER	PRO	engineered mutation	UNP Q00955
C	1762	LEU	ILE	engineered mutation	UNP Q00955

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1765	VAL	MET	engineered mutation	UNP Q00955
C	1919	GLN	GLU	engineered mutation	UNP Q00955
C	1920	ALA	PRO	engineered mutation	UNP Q00955
C	1925	PHE	HIS	engineered mutation	UNP Q00955
C	2028	GLU	GLN	engineered mutation	UNP Q00955
C	2030	THR	MET	engineered mutation	UNP Q00955
C	2032	GLU	GLY	engineered mutation	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 2'-tert-butyl-1-(2H-indazol-5-ylcarbonyl)-2'H-spiro[piperidine-4,5'-pyrano[3,2-c]pyrazol]-7'(6'H)-one (three-letter code: 3W2) (formula: $C_{22}H_{25}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	30	22	5	3	0	0
			Total	C	N	O		
2	C	1	30	22	5	3	0	0

- Molecule 3 is water.

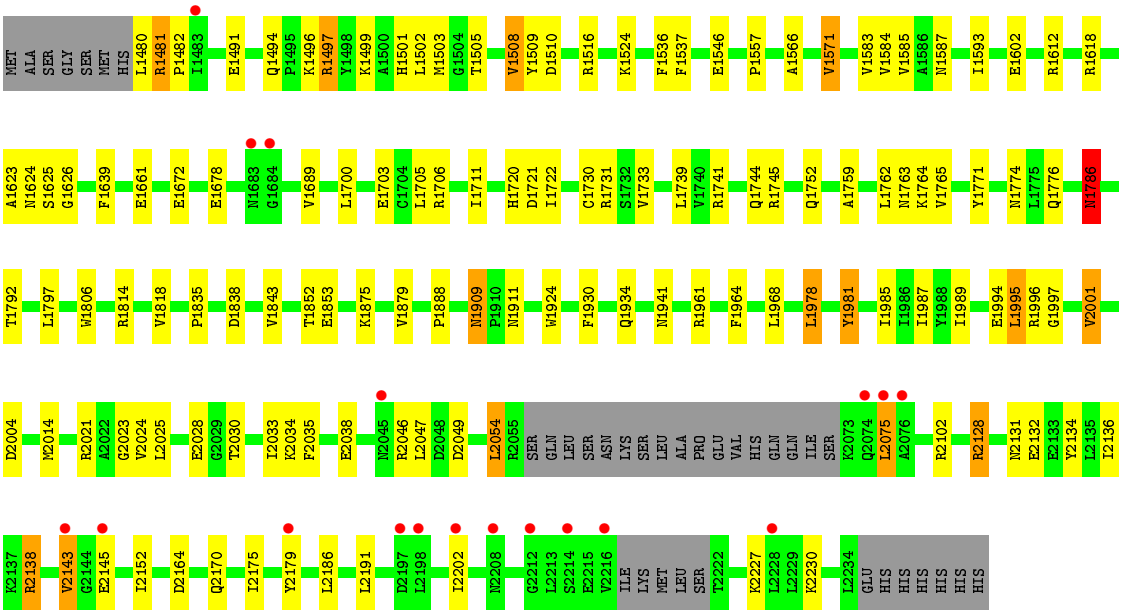
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	284	284	284	0	0
			Total	O		
3	C	263	263	263	0	0

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 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.

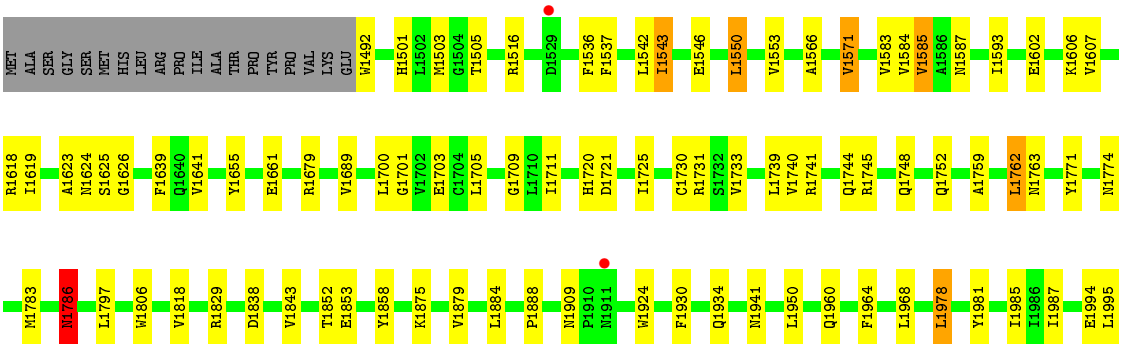
- Molecule 1: Acetyl-CoA carboxylase

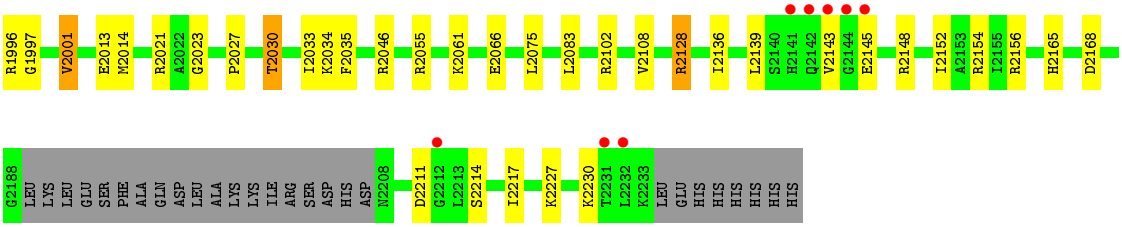
Chain B:



- Molecule 1: Acetyl-CoA carboxylase

Chain C:




R1996
G1997
V2001
E2013
M2014
R2021
A2022
G2023
P2027
T2030
I2033
K2034
F2035
R2046
R2055
K2061
E2066
L2075
L2083
R2102
V2108
R2128
I2136
L2139
S2140
H2141
Q2142
V2143
G2144
E2145
R2148
I2152
A2153
R2154
I2155
R2156
H2165
D2168
G2188
LEU
LYS
LEU
GLU
SER
PHE
ALA
GLN
ASP
LEU
ALA
LYS
LYS
ILE
ARG
SER
ASP
HIS
ASP
N2208
D2211
G2212
L2213
S2214
I2217
K2227
K2230
T2231
L2232
K2233
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.39Å 137.79Å 184.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.31 – 2.89 42.02 – 2.89	Depositor EDS
% Data completeness (in resolution range)	89.3 (42.31-2.89) 89.3 (42.02-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.90Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.5	Depositor
R, R_{free}	0.154 , 0.207 0.160 , 0.216	Depositor DCC
R_{free} test set	2412 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 64.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12185	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, 0.333 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: 3W2

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	B	0.52	0/5958	0.73	1/8066 (0.0%)
1	C	0.52	0/5862	0.74	1/7936 (0.0%)
All	All	0.52	0/11820	0.74	2/16002 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1786	ASN	CB-CA-C	-5.59	99.22	110.40
1	C	1786	ASN	CB-CA-C	-5.41	99.57	110.40

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	B	5834	0	5756	69	0
1	C	5744	0	5663	62	0
2	B	30	0	25	1	0
2	C	30	0	25	1	0
3	B	284	0	0	5	0
3	C	263	0	0	4	0
All	All	12185	0	11469	116	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 5.

The worst 5 of 116 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:1763:ASN:HD21	1:B:1771:TYR:H	1.22	0.82
1:C:1763:ASN:HD21	1:C:1771:TYR:H	1.24	0.82
1:B:2046:ARG:NH2	1:C:1639:PHE:O	2.20	0.73
1:B:1741:ARG:HH22	1:B:1934:GLN:HE22	1.36	0.73
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.40	0.70

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	B	728/769 (95%)	695 (96%)	28 (4%)	5 (1%)	22	54
1	C	719/769 (94%)	689 (96%)	25 (4%)	5 (1%)	22	54
All	All	1447/1538 (94%)	1384 (96%)	53 (4%)	10 (1%)	22	54

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1744	GLN
1	B	1875	LYS
1	C	1744	GLN
1	C	1875	LYS
1	B	2143	VAL

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	B	616/658 (94%)	564 (92%)	52 (8%)	11	31
1	C	610/658 (93%)	566 (93%)	44 (7%)	14	39
All	All	1226/1316 (93%)	1130 (92%)	96 (8%)	12	34

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2049	ASP
1	C	1516	ARG
1	C	2061	LYS
1	B	2054	LEU
1	B	2143	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2170	GLN
1	C	1599	GLN
1	C	2068	HIS
1	C	1517	GLN
1	C	1522	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	3W2	B	4000	-	28,34,34	1.73	5 (17%)	32,53,53	1.22	3 (9%)
2	3W2	C	4000	-	28,34,34	1.58	5 (17%)	32,53,53	1.06	2 (6%)

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	3W2	B	4000	-	-	0/14/40/40	0/5/5/5
2	3W2	C	4000	-	-	3/14/40/40	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4000	3W2	C23-N24	-6.27	1.30	1.35
2	C	4000	3W2	C23-N24	-5.35	1.31	1.35
2	C	4000	3W2	C19-C18	2.48	1.46	1.40
2	C	4000	3W2	C8-C1	2.46	1.55	1.53
2	C	4000	3W2	C8-C9	2.39	1.54	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4000	3W2	C2-C1-C6	2.78	113.15	109.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4000	3W2	O7-C1-C8	2.54	112.78	109.64
2	B	4000	3W2	C5-N4-C3	2.23	116.92	112.62
2	C	4000	3W2	C2-C3-N4	-2.23	106.52	110.92
2	C	4000	3W2	C12-C11-N4	2.11	121.39	118.72

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4000	3W2	C28-C27-N25-N24
2	C	4000	3W2	C29-C27-N25-N24
2	C	4000	3W2	C30-C27-N25-N24

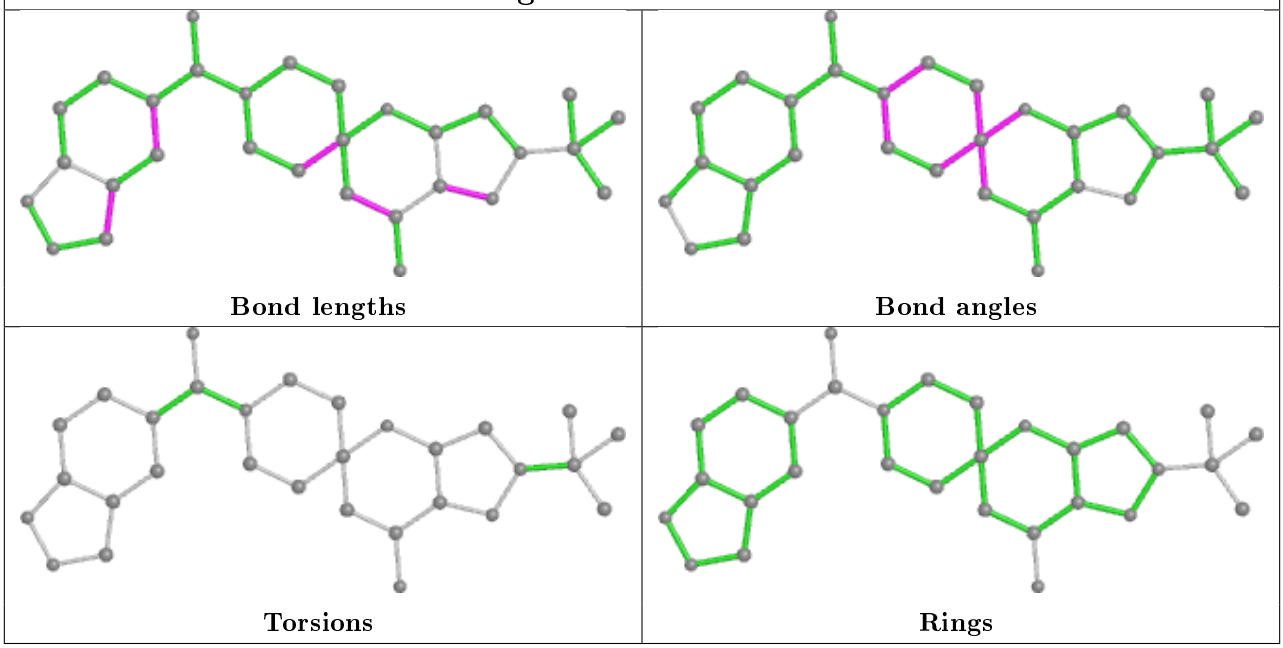
There are no ring outliers.

2 monomers are involved in 2 short contacts:

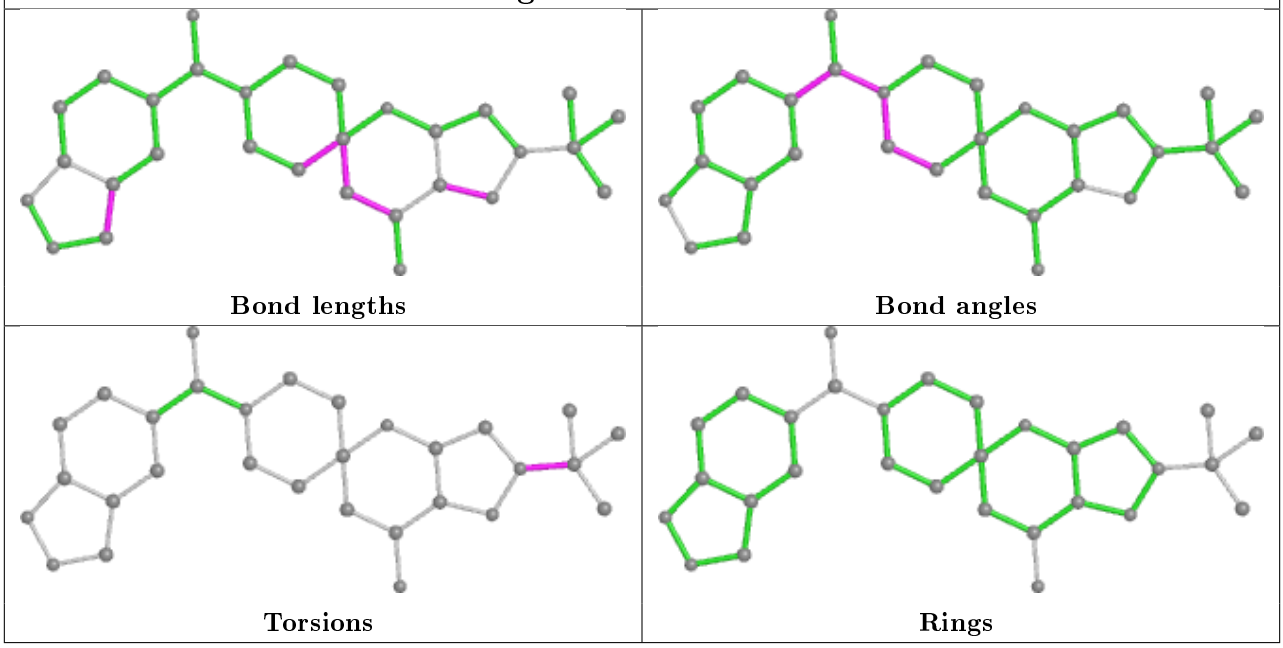
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4000	3W2	1	0
2	C	4000	3W2	1	0

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 then 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.

Ligand 3W2 B 4000



Ligand 3W2 C 4000



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	B	733/769 (95%)	-0.35	18 (2%)	57	55	20, 42, 92, 118	0
1	C	723/769 (94%)	-0.49	10 (1%)	75	75	18, 42, 77, 107	0
All	All	1456/1538 (94%)	-0.42	28 (1%)	66	65	18, 42, 85, 118	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2144	GLY	4.3
1	C	2143	VAL	4.0
1	B	2074	GLN	3.2
1	C	2145	GLU	3.1
1	C	2141	HIS	3.0

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)

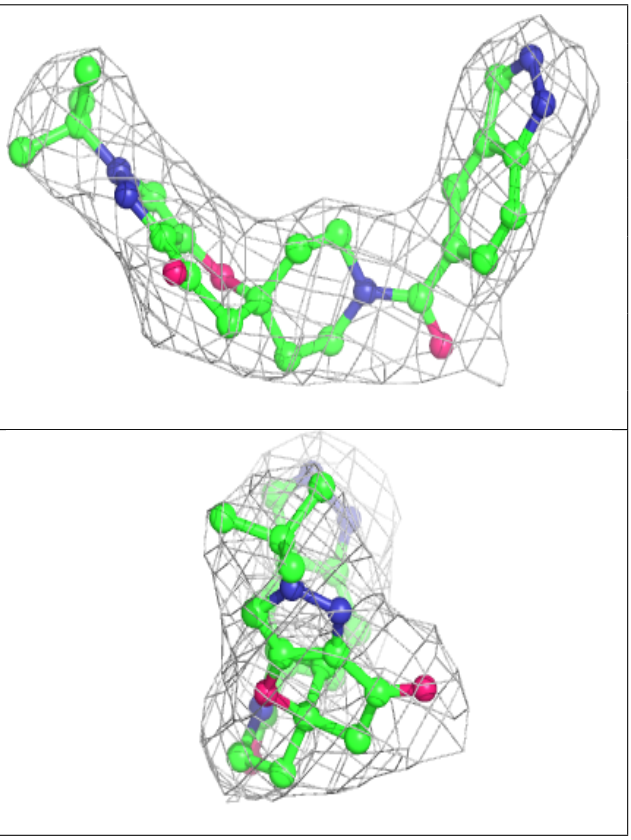
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	3W2	B	4000	30/30	0.97	0.14	33,38,45,45	0
2	3W2	C	4000	30/30	0.98	0.14	19,33,41,42	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.

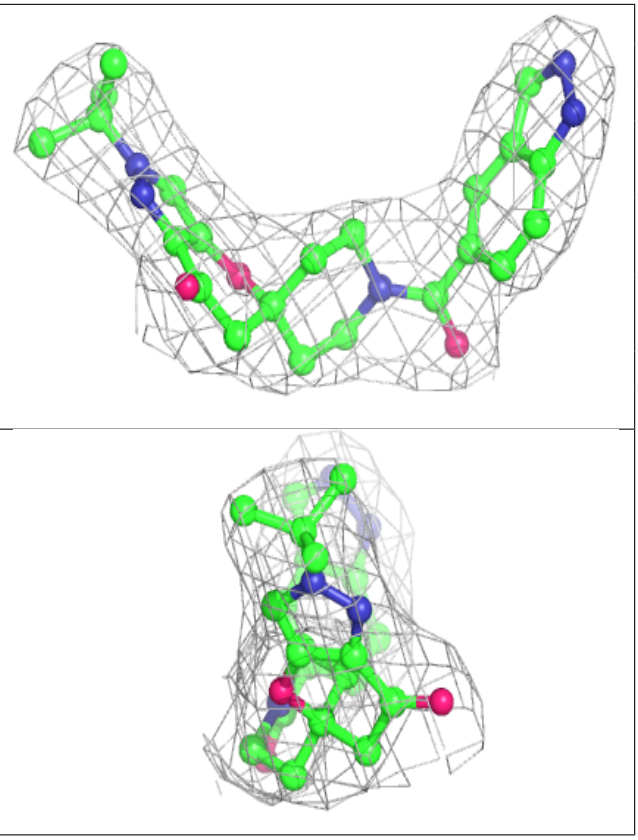
Electron density around 3W2 B 4000:

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 3W2 C 4000:

$2mF_o$-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.