wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2026 – 10:19 AM EDT

PDB ID	:	9YV2 / pdb_00009yv2
Title	:	Crystal structure of the human DCAF1 WDR domain in complex with OICR-40151
Authors	:	kimani, S.; Dong, A.; Li, Y.; Seitova, A.; Mamai, A.; Al-awar, R.; Ackloo, S.; Arrowsmith, C.H.; Edwards, A.M.; Halabelian, L.; Structural Genomics Consortium (SGC)
Deposited on	:	2025-10-23
Resolution	:	1.67 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

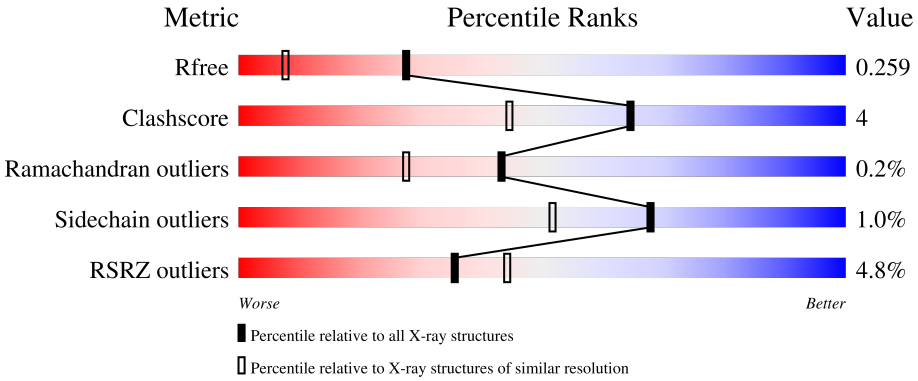
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.67 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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 <=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	315	4% 88% 7% •
1	B	315	5% 85% 8% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5372 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.

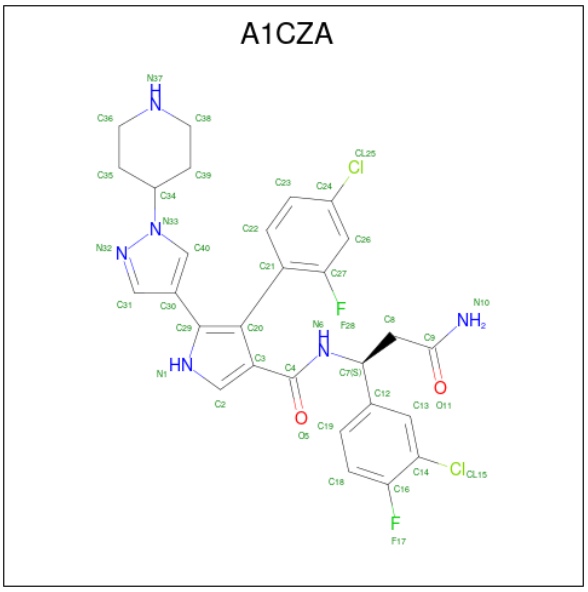
- Molecule 1 is a protein called DDB1- and CUL4-associated factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	11	0
			2431	1533	408	470	20			
1	B	297	Total	C	N	O	S	0	9	1
			2376	1511	404	444	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1076	GLY	-	expression tag	UNP Q9Y4B6
A	1077	ALA	-	expression tag	UNP Q9Y4B6
A	1078	SER	-	expression tag	UNP Q9Y4B6
A	1079	ALA	-	expression tag	UNP Q9Y4B6
B	1076	GLY	-	expression tag	UNP Q9Y4B6
B	1077	ALA	-	expression tag	UNP Q9Y4B6
B	1078	SER	-	expression tag	UNP Q9Y4B6
B	1079	ALA	-	expression tag	UNP Q9Y4B6

- Molecule 2 is (4P,5M)-N-[(1S)-3-amino-1-(3-chloro-4-fluorophenyl)-3-oxopropyl]-4-(4-chloro-2-fluorophenyl)-5-[1-(piperidin-4-yl)-1H-pyrazol-4-yl]-1H-pyrrole-3-carboxamide (CCD ID: A1CZA) (formula: $C_{28}H_{26}Cl_2F_2N_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C Cl F N O 40 28 2 2 6 2	0	0
2	B	1	Total C Cl F N O 40 28 2 2 6 2	0	0

- Molecule 3 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total X 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	253	Total O 256 256	0	3
4	B	225	Total O 227 227	0	2

3 Residue-property plots (i)

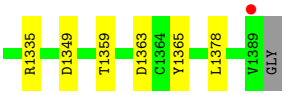
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DDB1- and CUL4-associated factor 1

Chain A:





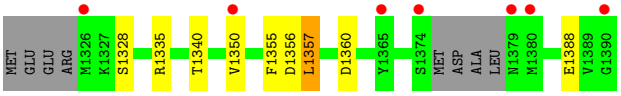


• Molecule 1: DDB1- and CUL4-associated factor 1

Chain B:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.79Å 88.66Å 73.39Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	18.76 – 1.67 18.76 – 1.67	Depositor EDS
% Data completeness (in resolution range)	95.0 (18.76-1.67) 95.1 (18.76-1.67)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.219 , 0.253 0.228 , 0.259	Depositor DCC
R_{free} test set	3447 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å^2)	17.6	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5372	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, A1CZA

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	0.59	0/2490	0.89	3/3380 (0.1%)
1	B	0.59	0/2444	0.91	3/3316 (0.1%)
All	All	0.59	0/4934	0.90	6/6696 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1218	ASP	CA-CB-CG	7.53	120.13	112.60
1	A	1314	GLN	CB-CA-C	7.49	122.15	109.80
1	A	1146	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	1356	ASP	CA-CB-CG	5.24	117.83	112.60
1	A	1349	ASP	CA-CB-CG	5.23	117.83	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1335	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	1081	ARG	Sidechain
1	B	1247[A]	ARG	Sidechain

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	2431	0	2293	17	0
1	B	2376	0	2266	20	0
2	A	40	0	0	1	0
2	B	40	0	0	1	0
3	A	2	0	0	0	0
4	A	256	0	0	5	0
4	B	227	0	0	7	0
All	All	5372	0	4559	37	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 4.

The worst 5 of 37 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:1181:TYR:OH	1:A:1225[A]:ARG:NH1	1.74	1.18
1:A:1312:MET:HE2	4:A:1546:HOH:O	1.78	0.82
1:A:1359[B]:THR:HG23	1:A:1365:TYR:O	1.79	0.81
1:B:1181:TYR:CD2	1:B:1227[A]:CYS:SG	2.81	0.74
1:A:1227[B]:CYS:SG	2:A:1401:A1CZA:CL25	2.85	0.72

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	309/315 (98%)	301 (97%)	8 (3%)	0	100 100
1	B	298/315 (95%)	288 (97%)	9 (3%)	1 (0%)	36 21
All	All	607/630 (96%)	589 (97%)	17 (3%)	1 (0%)	43 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1080	PHE

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	A	268/276 (97%)	267 (100%)	1 (0%)	84 78
1	B	259/276 (94%)	255 (98%)	4 (2%)	57 34
All	All	527/552 (96%)	522 (99%)	5 (1%)	68 55

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1259	ASN
1	B	1106	ARG
1	B	1259	ASN
1	B	1350	VAL
1	B	1357	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1353	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are unknown - leaving 2 for Mogul analysis.

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	A1CZA	A	1401	-	44,44,44	0.49	0	55,63,63	0.69	2 (3%)
2	A1CZA	B	1401	-	44,44,44	0.44	0	55,63,63	0.67	1 (1%)

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	A1CZA	A	1401	-	-	3/28/36/36	0/5/5/5
2	A1CZA	B	1401	-	-	4/28/36/36	0/5/5/5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1401	A1CZA	C39-C34-N33	3.26	115.42	110.95
2	A	1401	A1CZA	C39-C34-N33	-2.75	107.19	110.95
2	A	1401	A1CZA	C34-N33-N32	-2.32	117.24	120.41

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	A1CZA	N1-C29-C30-C31
2	A	1401	A1CZA	C20-C29-C30-C31
2	B	1401	A1CZA	N1-C29-C30-C31
2	B	1401	A1CZA	C20-C29-C30-C31
2	B	1401	A1CZA	C20-C29-C30-C40

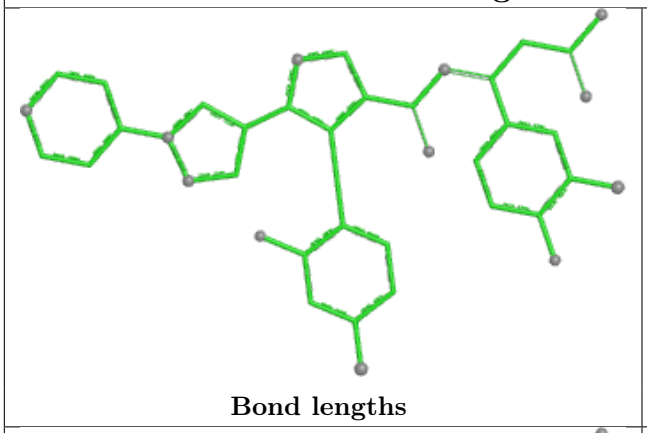
There are no ring outliers.

2 monomers are involved in 2 short contacts:

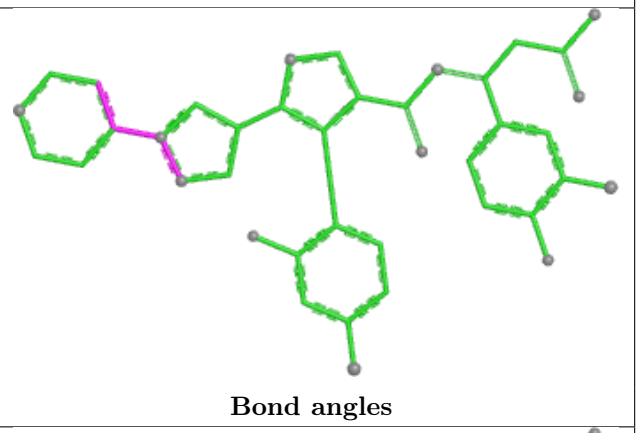
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	A1CZA	1	0
2	B	1401	A1CZA	1	0

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.

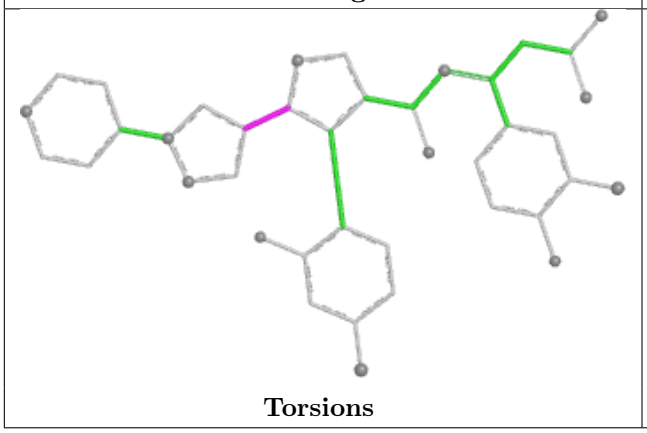
Ligand A1CZA A 1401



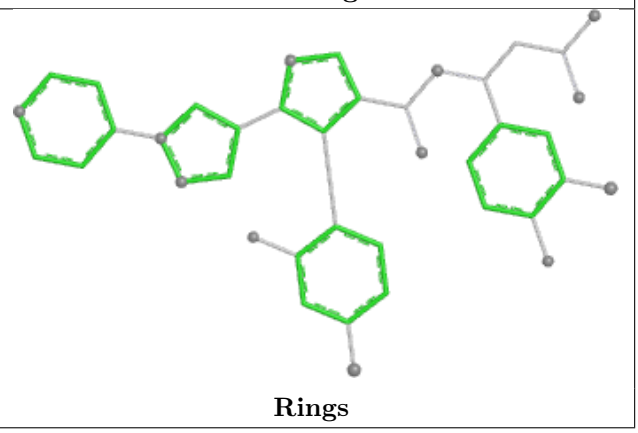
Bond lengths



Bond angles

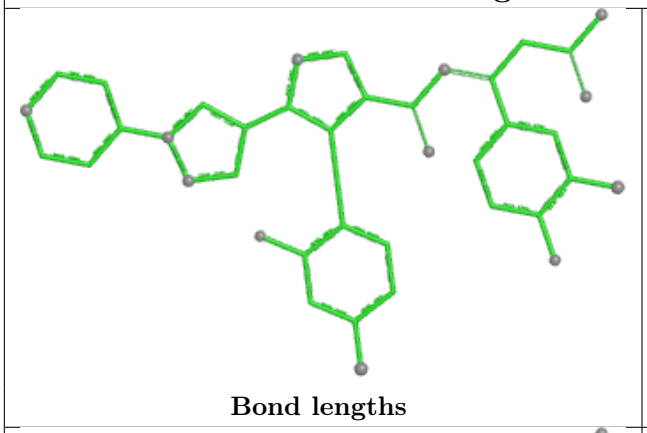


Torsions

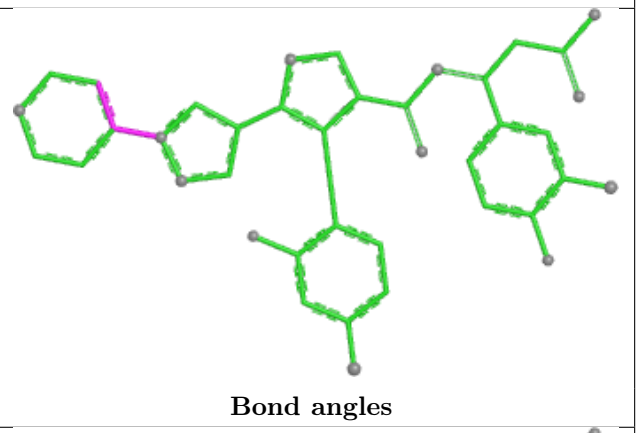


Rings

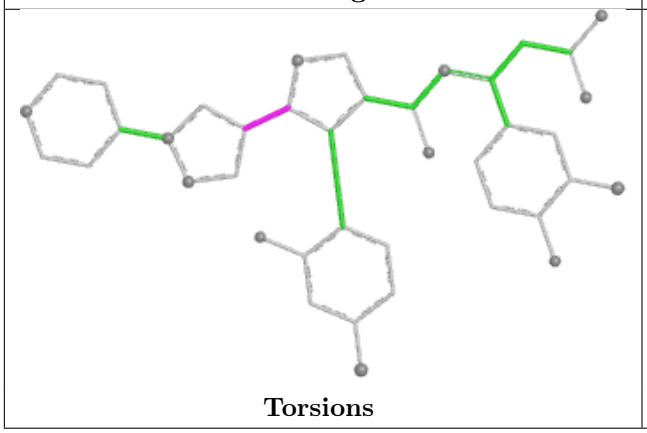
Ligand A1CZA B 1401



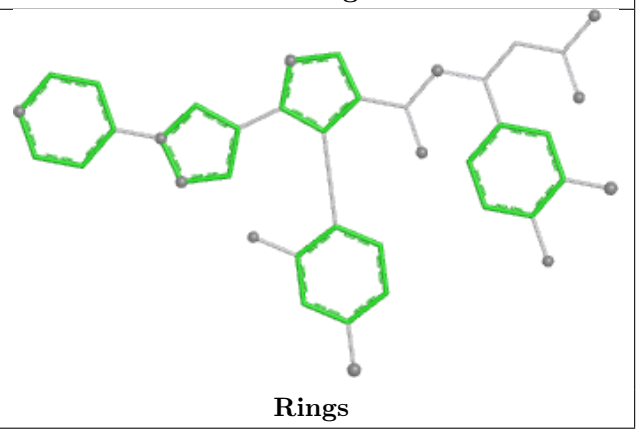
Bond lengths



Bond angles



Torsions



Rings

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	301/315 (95%)	0.24	12 (3%)	42	50	5, 17, 35, 50	11 (3%)
1	B	297/315 (94%)	0.33	17 (5%)	29	38	6, 19, 37, 55	9 (3%)
All	All	598/630 (94%)	0.28	29 (4%)	35	44	5, 18, 37, 55	20 (3%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1390	GLY	5.1
1	B	1079	ALA	5.0
1	B	1156	TRP	4.1
1	B	1107	PHE	3.8
1	A	1079	ALA	3.6

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 oligosaccharides in this entry.

6.4 Ligands

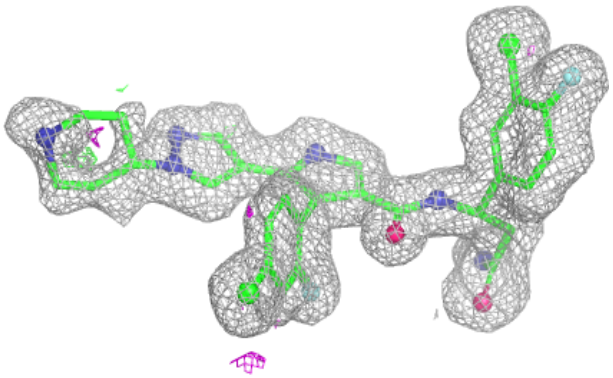
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

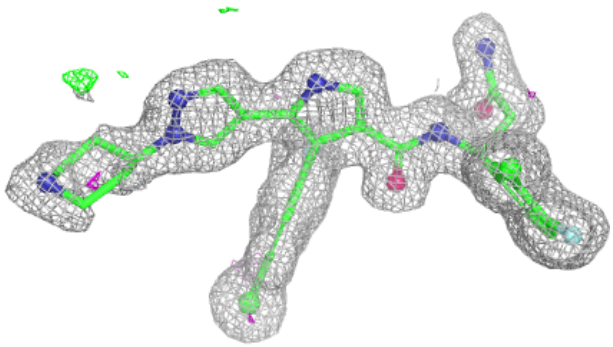
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	UNX	A	1403	1/1	0.95	0.13	1,1,1,1	0
3	UNX	A	1402	1/1	0.96	0.21	0,0,0,0	0
2	A1CZA	B	1401	40/40	0.96	0.08	14,17,34,36	0
2	A1CZA	A	1401	40/40	0.97	0.07	11,13,32,33	0

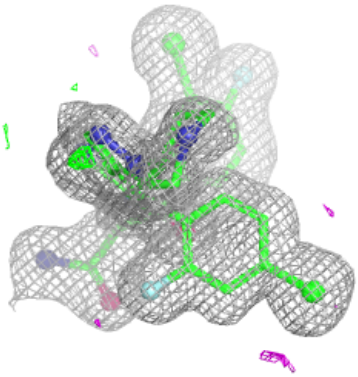
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1CZA B 1401:

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

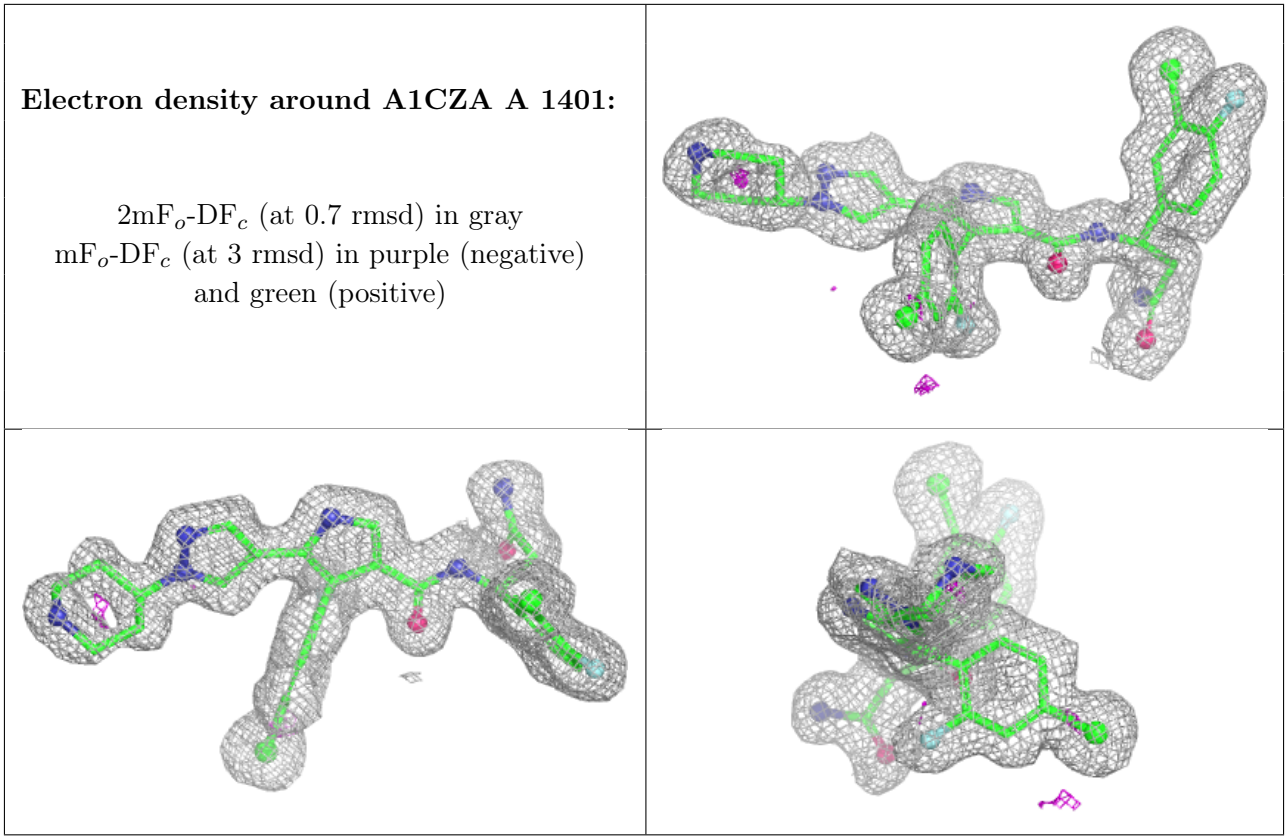






Electron density around A1CZA A 1401:

$2mF_o$-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.