Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 07:16 am GMT

PDB ID	:	2W6N
Title	:	Crystal structure of Biotin carboxylase from E. coli in complex with amino-oxazole fragment series
Authors	:	Mochalkin, I.; Miller, J.R.
Deposited on	:	2008-12-18
Resolution	:	1.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i)) were used in the production of this report:

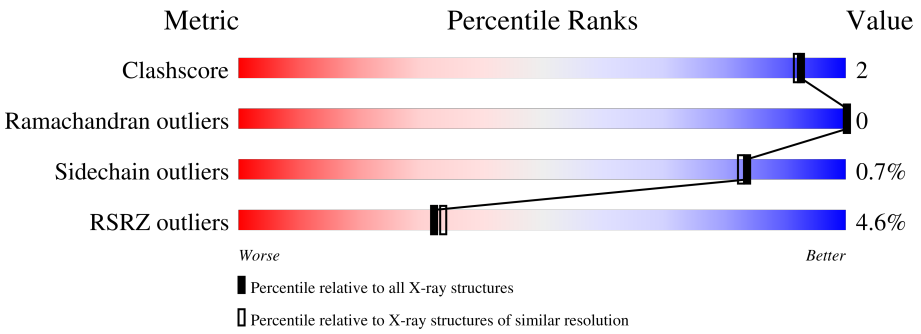
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.87 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	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	449	96%
1	B	449	9% 95%

2 Entry composition (i)

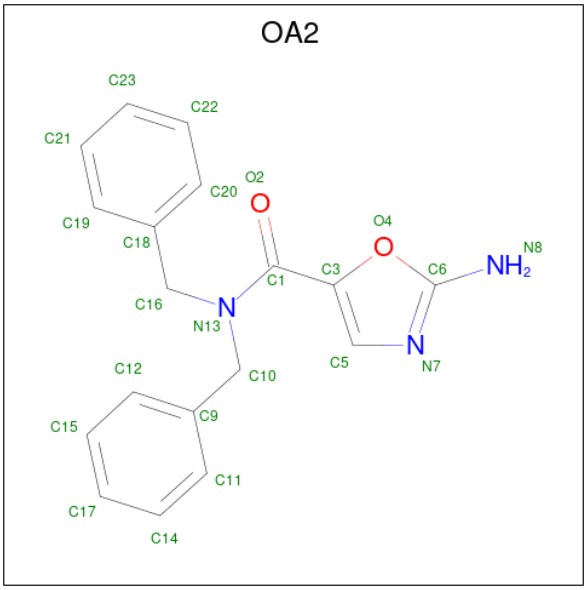
There are 4 unique types of molecules in this entry. The entry contains 7959 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BIOTIN CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	445	3425	2157	612	634	22	0	0	0
1	B	445	3425	2157	612	634	22	0	0	0

- Molecule 2 is 2-AMINO-N,N-BIS(PHENYLMETHYL)-1,3-OXAZOLE-5-CARBOXAMIDE (three-letter code: OA2) (formula: $C_{18}H_{17}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	23	18	3	2	0	0
2	B	1	23	18	3	2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	1	1	1	0	0
			Total	Cl		
3	B	1	1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	598	598	598	0	0
			Total	O		
4	B	463	463	463	0	0

3 Residue-property plots (i)

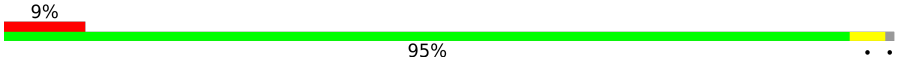
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

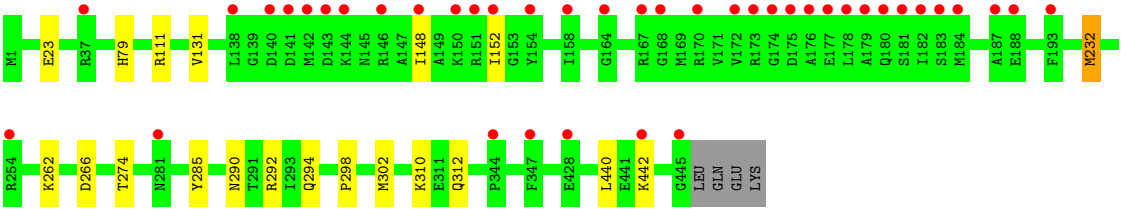
• Molecule 1: BIOTIN CARBOXYLASE

Chain A:

• Molecule 1: BIOTIN CARBOXYLASE

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.14Å 105.94Å 122.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.06 – 1.87 49.51 – 1.87	Depositor EDS
% Data completeness (in resolution range)	95.0 (80.06-1.87) 90.4 (49.51-1.87)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.175 , 0.217 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7959	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: CL, OA2

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	0.44	0/3488	0.60	2/4707 (0.0%)
1	B	0.44	0/3488	0.59	0/4707
All	All	0.44	0/6976	0.60	2/9414 (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	A	314	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	314	ARG	NE-CZ-NH1	5.30	122.95	120.30

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	3425	0	3448	6	0
1	B	3425	0	3448	14	0
2	A	23	0	17	0	0
2	B	23	0	17	1	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
4	A	598	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	463	0	0	1	0
All	All	7959	0	6930	21	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 2.

All (21) 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:232:MET:HE2	1:B:440:LEU:HB2	1.75	0.68
1:A:79:HIS:HD1	1:A:81:GLY:H	1.45	0.64
1:A:340:ASN:HD22	1:A:384:MET:HA	1.63	0.64
1:B:232:MET:CE	1:B:440:LEU:HB2	2.31	0.59
1:B:292:ARG:NH1	3:B:1447:CL:CL	2.75	0.56
1:B:274:THR:HG21	1:B:294:GLN:HE22	1.72	0.54
1:B:232:MET:HE3	4:B:2455:HOH:O	2.09	0.52
1:B:23:GLU:OE1	1:B:310:LYS:CE	2.59	0.49
1:B:79:HIS:HE2	1:B:312:GLN:NE2	2.12	0.47
1:B:131:VAL:HG22	1:B:285:TYR:HB3	1.97	0.47
1:B:262:LYS:NZ	1:B:266:ASP:OD1	2.45	0.47
1:B:232:MET:CE	1:B:232:MET:HA	2.46	0.46
2:B:1446:OA2:H102	2:B:1446:OA2:H5	1.99	0.45
1:A:314:ARG:HD3	4:A:2458:HOH:O	2.18	0.43
1:B:290:ASN:ND2	1:B:294:GLN:OE1	2.52	0.43
1:B:148:ILE:HG22	1:B:152:ILE:HD12	2.01	0.43
1:A:1:MET:HE3	1:A:2:LEU:H	1.84	0.43
1:B:23:GLU:OE1	1:B:310:LYS:NZ	2.50	0.41
1:A:404:ASN:ND2	4:A:2552:HOH:O	2.53	0.41
1:A:298:PRO:O	1:A:302:MET:HG2	2.22	0.40
1:B:298:PRO:O	1:B:302:MET:HG2	2.22	0.40

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	443/449 (99%)	435 (98%)	8 (2%)	0	100	100
1	B	443/449 (99%)	433 (98%)	10 (2%)	0	100	100
All	All	886/898 (99%)	868 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	357/361 (99%)	355 (99%)	2 (1%)	86	86
1	B	357/361 (99%)	354 (99%)	3 (1%)	81	80
All	All	714/722 (99%)	709 (99%)	5 (1%)	84	83

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

Mol	Chain	Res	Type
1	A	237	GLN
1	A	323	ILE
1	B	111	ARG
1	B	232	MET
1	B	442	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	206	ASN
1	A	312	GLN
1	A	319	GLN
1	A	340	ASN

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Mol	Chain	Res	Type
1	A	404	ASN
1	A	431	GLN
1	B	94	GLN
1	B	290	ASN
1	B	294	GLN
1	B	312	GLN
1	B	319	GLN
1	B	404	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - 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	OA2	B	1446	-	23,25,25	0.67	0	26,33,33	0.96	2 (7%)
2	OA2	A	1446	-	23,25,25	0.62	0	26,33,33	1.01	1 (3%)

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	OA2	B	1446	-	-	0/12/16/16	0/3/3/3
2	OA2	A	1446	-	-	0/12/16/16	0/3/3/3

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	1446	OA2	C3-C1-N13	2.38	125.88	119.81
2	A	1446	OA2	C3-C1-N13	2.15	125.31	119.81
2	B	1446	OA2	O2-C1-N13	-2.07	118.91	122.34

There are no chirality outliers.

There are no torsion outliers.

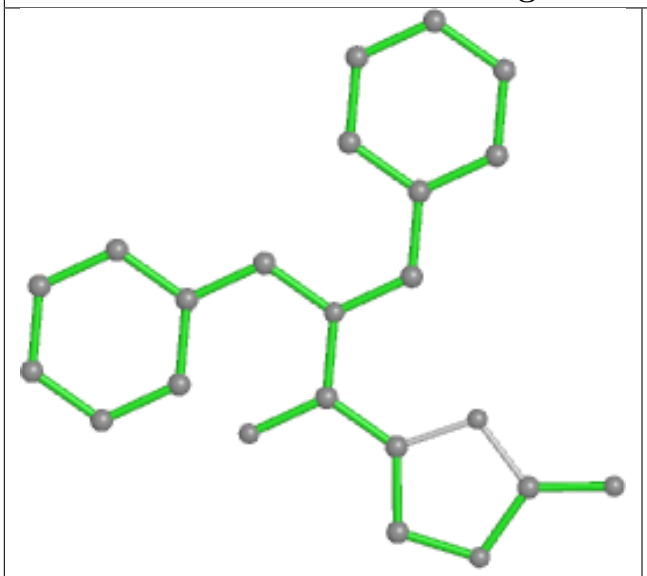
There are no ring outliers.

1 monomer is involved in 1 short contact:

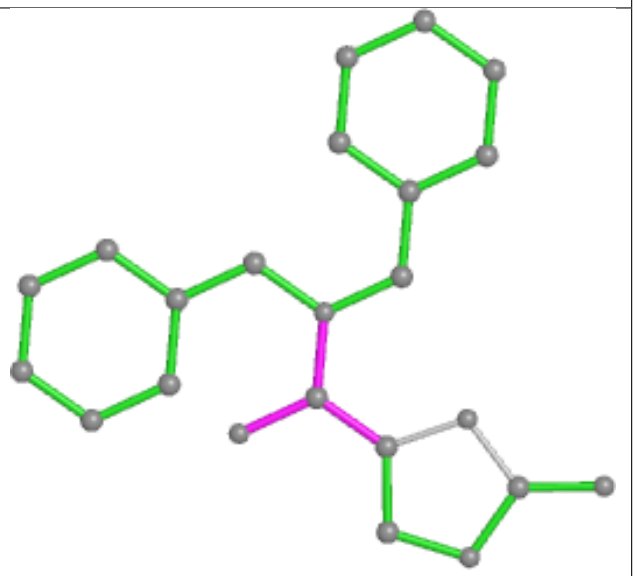
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1446	OA2	1	0

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.

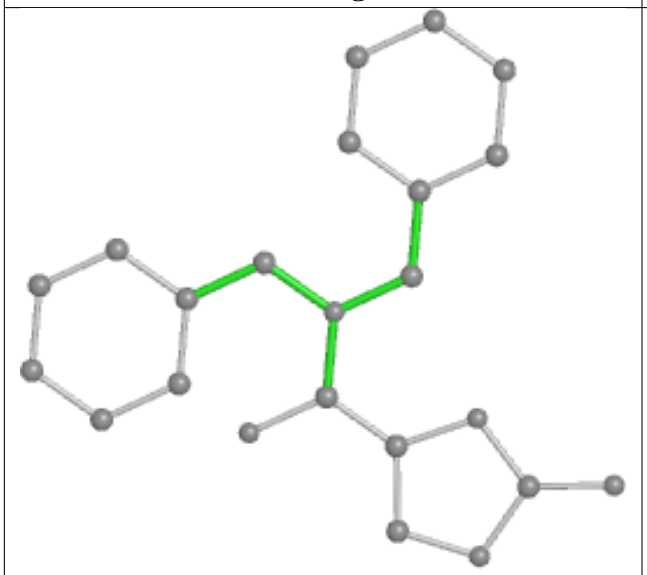
Ligand OA2 B 1446



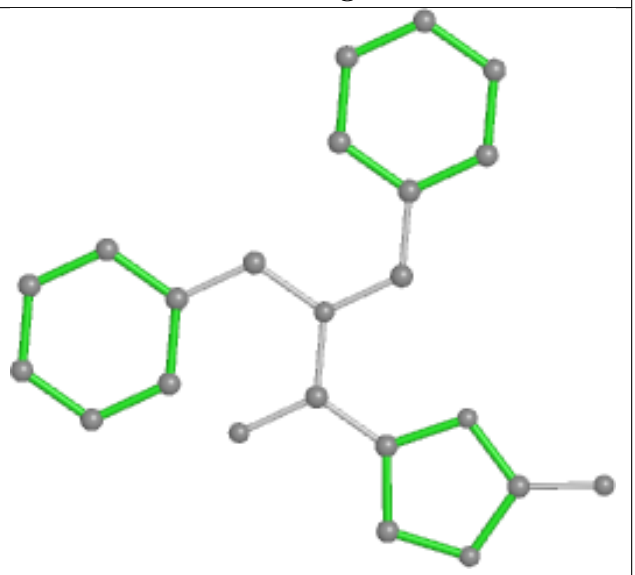
Bond lengths



Bond angles

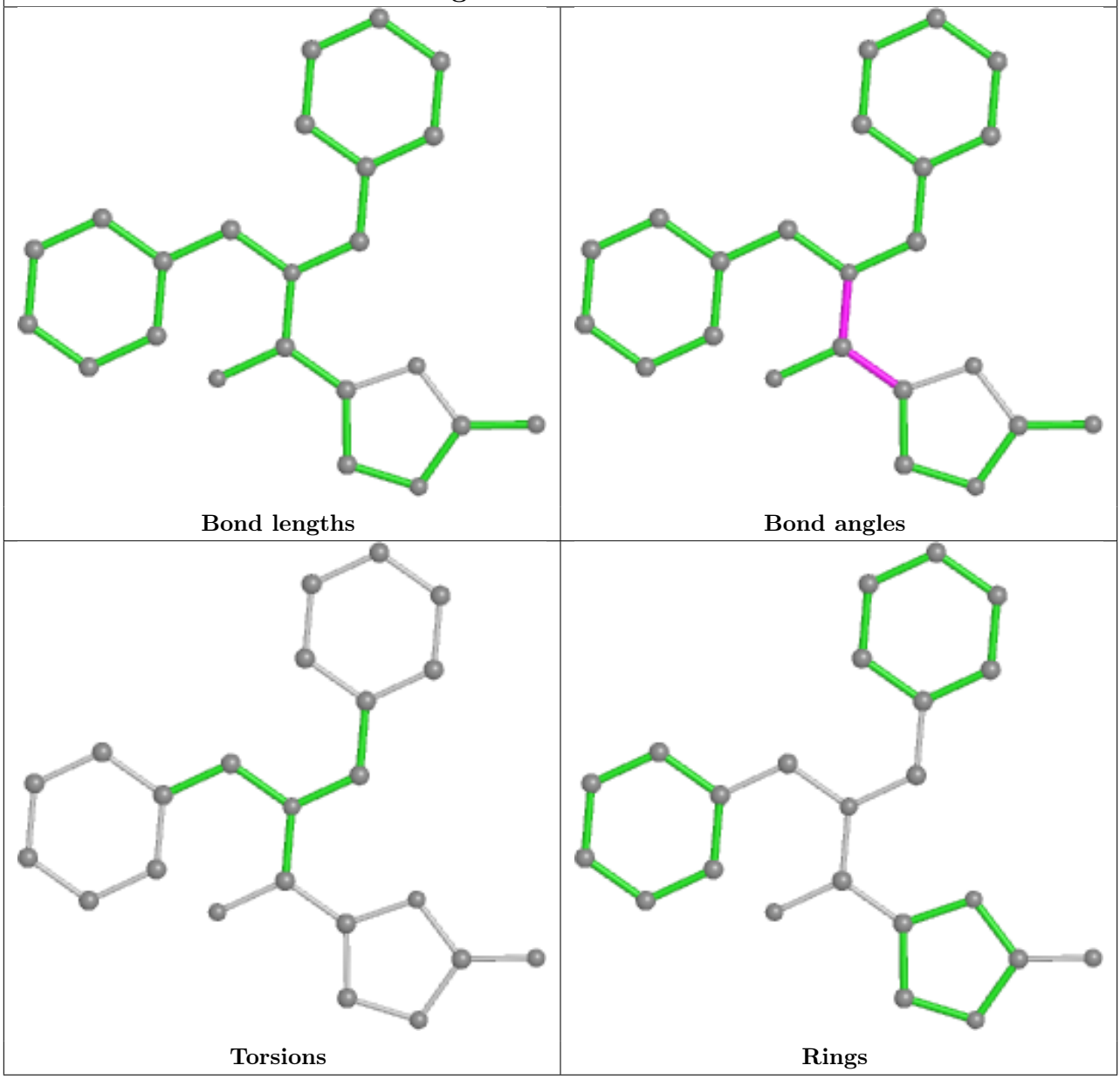


Torsions



Rings

Ligand OA2 A 1446



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	445/449 (99%)	-0.20	0 100 100	13, 18, 27, 34	3 (0%)
1	B	445/449 (99%)	0.35	41 (9%) 9 9	12, 19, 46, 52	4 (0%)
All	All	890/898 (99%)	0.08	41 (4%) 32 34	12, 18, 39, 52	7 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	MET	5.5
1	B	347	PHE	5.0
1	B	144	LYS	4.8
1	B	143	ASP	4.7
1	B	168	GLY	4.4
1	B	154	TYR	4.2
1	B	180	GLN	4.2
1	B	152	ILE	4.1
1	B	176	ALA	4.0
1	B	146	ARG	3.9
1	B	150	LYS	3.7
1	B	141	ASP	3.7
1	B	167	ARG	3.6
1	B	172	VAL	3.6
1	B	183	SER	3.5
1	B	344	PRO	3.5
1	B	140	ASP	3.5
1	B	174	GLY	3.2
1	B	178	LEU	3.2
1	B	173	ARG	3.2
1	B	179	ALA	3.2
1	B	177	GLU	3.1
1	B	184	MET	2.9
1	B	281	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	182	ILE	2.9
1	B	138	LEU	2.8
1	B	175	ASP	2.7
1	B	148	ILE	2.7
1	B	188	GLU	2.7
1	B	442	LYS	2.6
1	B	151	ARG	2.6
1	B	254	ARG	2.6
1	B	445	GLY	2.5
1	B	193	PHE	2.5
1	B	164	GLY	2.4
1	B	37	ARG	2.3
1	B	181	SER	2.2
1	B	170	ARG	2.2
1	B	187	ALA	2.1
1	B	158	ILE	2.1
1	B	428	GLU	2.1

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 monosaccharides 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.

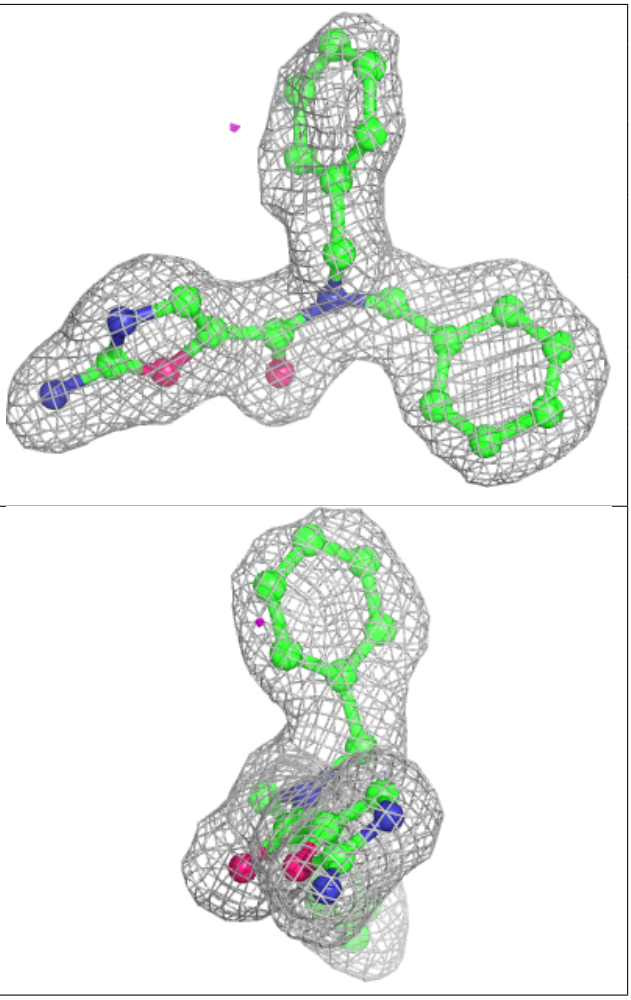
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OA2	B	1446	23/23	0.91	0.14	26,29,34,34	0
2	OA2	A	1446	23/23	0.96	0.08	15,20,21,21	0
3	CL	B	1447	1/1	0.99	0.09	24,24,24,24	0
3	CL	A	1447	1/1	1.00	0.11	17,17,17,17	0

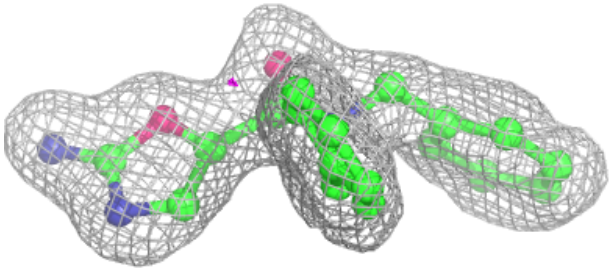
The following is a graphical depiction of the model fit to experimental electron density of all

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 OA2 B 1446:

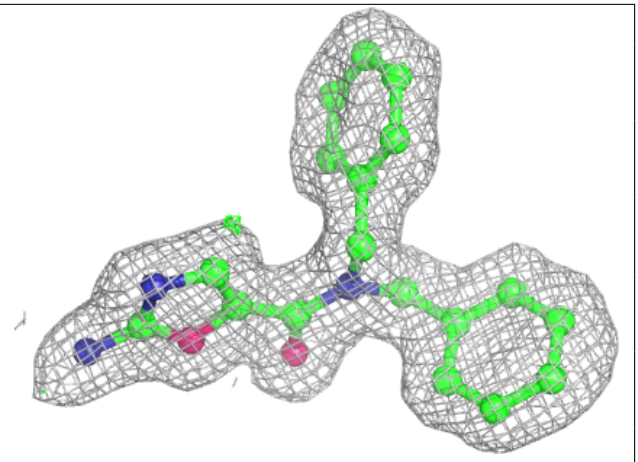
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

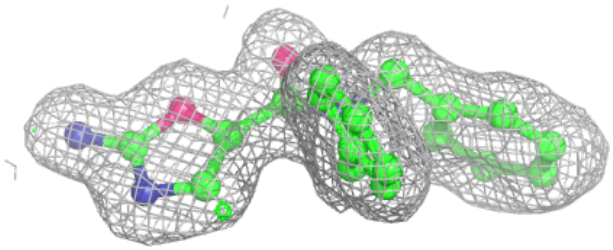


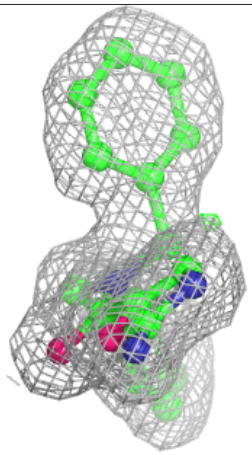


Electron density around OA2 A 1446:

$2mF_o$-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.