

Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 02:21 PM JST

PDB ID	:	8JI4
Title	:	Crystal structure of AetD in complex with 5-bromo-L-tryptophan
Authors	:	Li, H.; Dai, L.; Zheng, H.B.; Chen, CC.; Guo, RT.
Deposited on		
Resolution	:	1.67 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 (1)) were used in the production of this report:

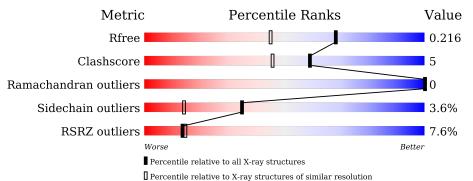
Xtriage (Phenix) EDS buster-report Percentile statistics	: : :	20191225.v01 (using entries in the PDB archive December 25th 2019)
-	:	
CCP4 Ideal geometry (proteins)		7.0.044 (Gargrove) Engh & Huber (2001)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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	А	249	88%	7%	•••
1	В	249	85%	10%	5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	TRS	А	307	-	-	Х	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4288 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	239	Total	С	Ν	0	S	0	1	0
	Л	239	1969	1255	339	367	8	0	1	0
1	В	236	Total	С	Ν	0	S	0	0	0
	D	230	1940	1238	331	363	8	0	U	0

• Molecule 1 is a protein called AetD.

Chain	Residue	Modelled	Actual	Comment	Reference
А	-9	ALA	-	expression tag	UNP A0A861B387
А	-8	GLY	-	expression tag	UNP A0A861B387
A	-7	ALA	-	expression tag	UNP A0A861B387
A	-6	GLY	-	expression tag	UNP A0A861B387
А	-5	ALA	-	expression tag	UNP A0A861B387
A	-4	GLY	-	expression tag	UNP A0A861B387
A	-3	ALA	-	expression tag	UNP A0A861B387
A	-2	GLY	-	expression tag	UNP A0A861B387
A	-1	ALA	-	expression tag	UNP A0A861B387
А	0	GLY	-	expression tag	UNP A0A861B387
В	-9	ALA	-	expression tag	UNP A0A861B387
В	-8	GLY	-	expression tag	UNP A0A861B387
В	-7	ALA	-	expression tag	UNP A0A861B387
В	-6	GLY	-	expression tag	UNP A0A861B387
В	-5	ALA	-	expression tag	UNP A0A861B387
В	-4	GLY	-	expression tag	UNP A0A861B387
В	-3	ALA	-	expression tag	UNP A0A861B387
В	-2	GLY	-	expression tag	UNP A0A861B387
В	-1	ALA	-	expression tag	UNP A0A861B387
В	0	GLY	-	expression tag	UNP A0A861B387

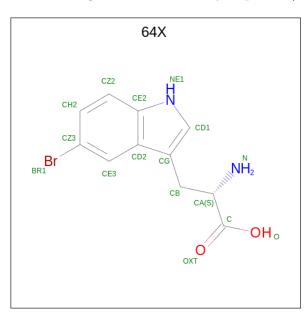
There are 20 discrepancies between the modelled and reference sequences:

• Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Fe 1 1	0	0
2	В	1	Total Fe 1 1	0	0

• Molecule 3 is 5-bromo-L-tryptophan (three-letter code: 64X) (formula: $C_{11}H_{11}BrN_2O_2$) (labeled as "Ligand of Interest" by depositor).



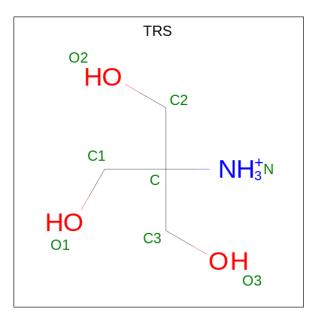
Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
2	Λ	1	Total	Br	С	Ν	Ο	0	0
5	A	1	16	1	11	2	2	0	0
2	В	1	Total	Br	С	Ν	Ο	0	0
3	D	1	16	1	11	2	2	0	0

• Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	3	Total Ni 3 3	0	0
4	В	2	Total Ni 2 2	0	0

• Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1, 3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 8 & 4 & 1 & 3 \end{array}$	0	0
5	А	1	Total C N O 8 4 1 3	0	0

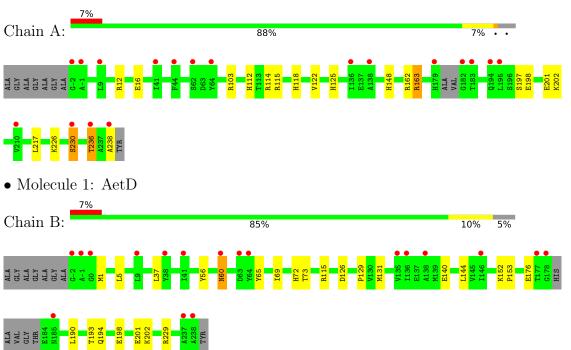
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	165	Total O 165 165	0	0
6	В	159	Total O 159 159	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: AetD



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants	65.42Å 65.42 Å 116.62 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.39 - 1.67	Depositor
Resolution (A)	23.38 - 1.67	EDS
% Data completeness	$99.5\ (23.39-1.67)$	Depositor
(in resolution range)	99.5(23.38-1.67)	EDS
R _{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.45 (at 1.67 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.172 , 0.207	Depositor
n, n _{free}	0.181 , 0.216	DCC
R_{free} test set	2768 reflections $(4.91%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	26.6	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34 , 41.0	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4288	wwPDB-VP
Average B, all atoms $(Å^2)$	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: FE2, NI, $64\mathrm{X},\,\mathrm{TRS}$

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	А	0.73	0/2013	0.90	3/2717~(0.1%)	
1	В	0.73	0/1980	0.88	1/2673~(0.0%)	
All	All	0.73	0/3993	0.89	4/5390~(0.1%)	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	114	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	А	103	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	А	114	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	В	56	TYR	CB-CG-CD1	5.33	124.20	121.00

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)	nodel) H(added)		Symm-Clashes
1	А	1969	0	1946	21	0
1	В	1940	0	1916	16	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	16	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	16	0	0	0	0
4	А	3	0	0	0	0
4	В	2	0	0	0	0
5	А	16	0	23	7	0
6	А	165	0	0	4	0
6	В	159	0	0	7	0
All	All	4288	0	3885	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 5.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:A:125:HIS:CE1	5:A:307:TRS:N	2.07	1.22
1:A:125:HIS:CE1	5:A:307:TRS:HN1	1.67	1.09
1:A:125:HIS:CE1	5:A:307:TRS:HN3	1.79	0.97
1:B:131:MET:HE1	1:B:202:LYS:HB3	1.68	0.76
1:A:125:HIS:HE1	5:A:307:TRS:HN3	1.31	0.74
1:B:140:GLU:OE2	6:B:401:HOH:O	2.07	0.72
1:A:125:HIS:HD1	5:A:307:TRS:H22	1.55	0.71
1:B:60:ASN:ND2	6:B:403:HOH:O	2.25	0.69
5:A:307:TRS:O3	1:B:126:ASP:OD2	2.12	0.66
1:A:118:HIS:HE1	6:B:441:HOH:O	1.79	0.64
1:B:65:TYR:HB2	1:B:129:PRO:HB2	1.88	0.56
1:A:163:ARG:HH21	1:A:236:THR:HG23	1.72	0.55
1:A:230:SER:O	1:A:230:SER:OG	2.23	0.54
1:A:112:HIS:HD2	6:A:521:HOH:O	1.93	0.52
1:A:163:ARG:NH2	1:A:236:THR:HG23	2.25	0.51
1:A:148:HIS:CE1	6:A:534:HOH:O	2.64	0.51
1:A:118:HIS:HD2	6:B:430:HOH:O	1.94	0.49
1:A:122:VAL:O	1:A:125:HIS:HD2	1.93	0.49
1:B:72:HIS:CE1	6:B:488:HOH:O	2.66	0.48
1:B:1:MET:HE2	1:B:5:LEU:HD21	1.96	0.48
1:A:226:LYS:CE	1:A:226:LYS:HA	2.44	0.48
1:B:131:MET:CE	1:B:202:LYS:HB3	2.43	0.46
1:B:1:MET:HG2	1:B:190:LEU:O	2.16	0.46
1:B:69:ILE:O	1:B:73:THR:HG23	2.15	0.46
1:B:115:ARG:NE	6:B:412:HOH:O	2.44	0.46
1:B:144:LEU:HD21	1:B:176:GLU:HB2	1.99	0.45
1:A:115[B]:ARG:NH1	6:A:403:HOH:O	2.39	0.44



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:HIS:ND1	5:A:307:TRS:N	2.41	0.43
1:A:163:ARG:HD3	1:A:238:ALA:HB2	2.01	0.43
1:B:1:MET:HE2	1:B:5:LEU:CD2	2.49	0.43
1:B:176:GLU:OE1	6:B:401:HOH:O	2.21	0.43
1:A:226:LYS:HA	1:A:226:LYS:HE3	2.01	0.42
1:A:12:ARG:O	1:A:16:GLU:HG3	2.19	0.42
1:B:152:LYS:HB2	1:B:153:PRO:CD	2.50	0.42
1:A:148:HIS:NE2	6:A:401:HOH:O	2.21	0.41
1:B:1:MET:CE	1:B:5:LEU:HG	2.50	0.41
1:A:217:LEU:C	1:A:217:LEU:HD23	2.41	0.41

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	А	236/249~(95%)	234~(99%)	2(1%)	0	100 100
1	В	232/249~(93%)	229~(99%)	3~(1%)	0	100 100
All	All	468/498~(94%)	463 (99%)	5 (1%)	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	А	212/213~(100%)	204~(96%)	8 (4%)	33 12	
1	В	209/213~(98%)	202~(97%)	7 (3%)	38 16	
All	All	421/426~(99%)	406 (96%)	15 (4%)	35 14	

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	162	ARG
1	А	163	ARG
1	А	197	SER
1	А	198	GLU
1	А	201	GLU
1	А	202	LYS
1	А	230	SER
1	А	236	THR
1	В	37	LEU
1	В	60	ASN
1	В	193	THR
1	В	194	GLN
1	В	198	GLU
1	В	201	GLU
1	В	229	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such side chains are listed below:

Mol	Chain	Res	Type
1	А	112	HIS
1	А	118	HIS
1	А	119	ASN
1	А	148	HIS
1	А	208	ASN
1	В	112	HIS
1	В	119	ASN
1	В	192	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	Turne	Type Chain Res		Res Link	Bond lengths			Bond angles						
WIOI	Type	Ullalli	nes	nes	nes	nes	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
5	TRS	А	307	-	7,7,7	0.17	0	9,9,9	0.44	0				
3	64X	В	302	2	$15,\!17,\!17$	2.10	6 (40%)	$17,\!24,\!24$	2.02	4 (23%)				
5	TRS	А	306	4	7,7,7	0.21	0	9,9,9	0.55	0				
3	64X	А	302	2	$15,\!17,\!17$	2.47	5 (33%)	$17,\!24,\!24$	<mark>3.73</mark>	<mark>6 (35%)</mark>				

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
5	TRS	А	307	-	-	7/9/9/9	-
3	64X	В	302	2	-	2/7/8/8	0/2/2/2
5	TRS	А	306	4	-	2/9/9/9	-
3	64X	А	302	2	-	1/7/8/8	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	302	64X	CE3-CZ3	7.03	1.47	1.36



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	В	302	64X	CE3-CZ3	4.22	1.43	1.36
3	В	302	64X	CZ2-CE2	-3.88	1.35	1.41
3	А	302	64X	BR1-CZ3	-3.22	1.83	1.90
3	В	302	64X	CE3-CD2	-3.12	1.35	1.42
3	А	302	64X	CD2-CE2	-2.66	1.35	1.42
3	А	302	64X	CE2-NE1	-2.60	1.30	1.38
3	А	302	64X	OXT-C	2.23	1.28	1.22
3	В	302	64X	CD2-CE2	-2.22	1.36	1.42
3	В	302	64X	CE2-NE1	-2.20	1.31	1.38
3	В	302	64X	CZ2-CH2	2.08	1.41	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	302	64X	BR1-CZ3-CH2	8.99	132.36	119.30
3	А	302	64X	CH2-CZ3-CE3	-8.57	110.04	121.99
3	А	302	64X	CZ2-CH2-CZ3	5.06	125.79	119.17
3	А	302	64X	CZ3-CE3-CD2	4.35	125.19	119.79
3	В	302	64X	CH2-CZ3-CE3	-4.34	115.94	121.99
3	А	302	64X	CB-CG-CD1	-4.31	122.64	127.97
3	В	302	64X	CB-CG-CD1	-4.28	122.68	127.97
3	В	302	64X	CZ2-CH2-CZ3	2.74	122.75	119.17
3	В	302	64X	CH2-CZ2-CE2	-2.55	117.63	120.84
3	А	302	64X	O-C-CA	2.28	121.16	113.38

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	306	TRS	N-C-C2-O2
5	А	307	TRS	N-C-C2-O2
5	А	307	TRS	C1-C-C3-O3
5	А	307	TRS	C2-C-C3-O3
5	А	307	TRS	C3-C-C2-O2
3	В	302	64X	N-CA-CB-CG
5	А	307	TRS	N-C-C1-O1
5	А	307	TRS	N-C-C3-O3
3	А	302	64X	N-CA-CB-CG
3	В	302	64X	C-CA-CB-CG
5	А	306	TRS	C3-C-C1-O1
5	А	307	TRS	C2-C-C1-O1



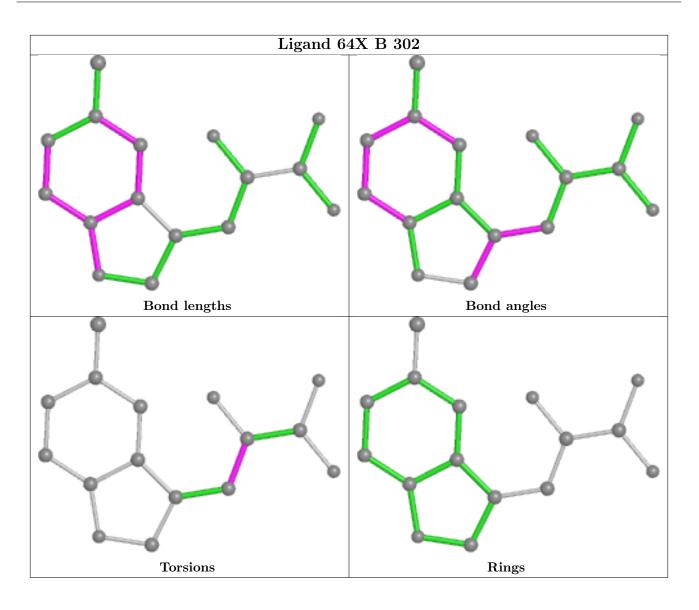
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	307	TRS	7	0

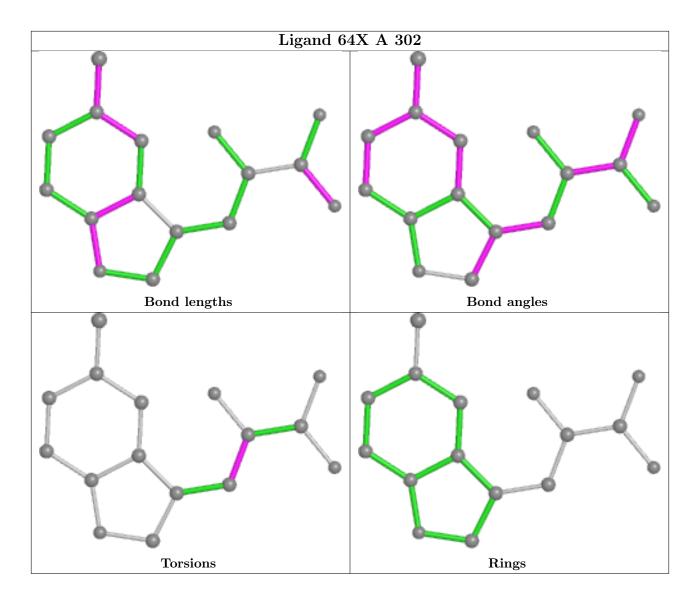
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











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, 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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	239/249~(95%)	0.31	18 (7%) 14 15	20, 31, 54, 76	0
1	В	236/249~(94%)	0.44	18 (7%) 13 15	20, 32, 59, 75	0
All	All	475/498~(95%)	0.37	36 (7%) 13 15	20, 31, 58, 76	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	-1	ALA	6.6
1	В	237	ALA	5.9
1	А	230	SER	5.8
1	В	238	ALA	5.5
1	В	-1	ALA	4.4
1	А	-2	GLY	3.8
1	В	-2	GLY	3.8
1	В	177	THR	3.7
1	А	183	THR	3.6
1	А	9	LEU	3.4
1	В	60	ASN	3.3
1	В	136	ILE	3.2
1	А	238	ALA	3.1
1	В	135	VAL	3.1
1	В	9	LEU	2.9
1	А	64	TYR	2.9
1	А	179	HIS	2.9
1	А	195	LEU	2.8
1	А	136	ILE	2.6
1	В	64	TYR	2.6
1	В	0	GLY	2.5
1	А	62	SER	2.5
1	А	182	GLY	2.4
1	В	41	ILE	2.4



Mol	Chain	Res	Type	RSRZ
1	А	194	GLN	2.4
1	В	138	ALA	2.4
1	В	185	ASN	2.4
1	В	178	GLY	2.4
1	А	236	THR	2.4
1	В	146	ILE	2.2
1	В	38	TYR	2.2
1	А	210	VAL	2.2
1	А	41	ILE	2.2
1	А	138	ALA	2.0
1	В	63	ASP	2.0
1	А	44	PHE	2.0

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 monosaccharides in this entry.

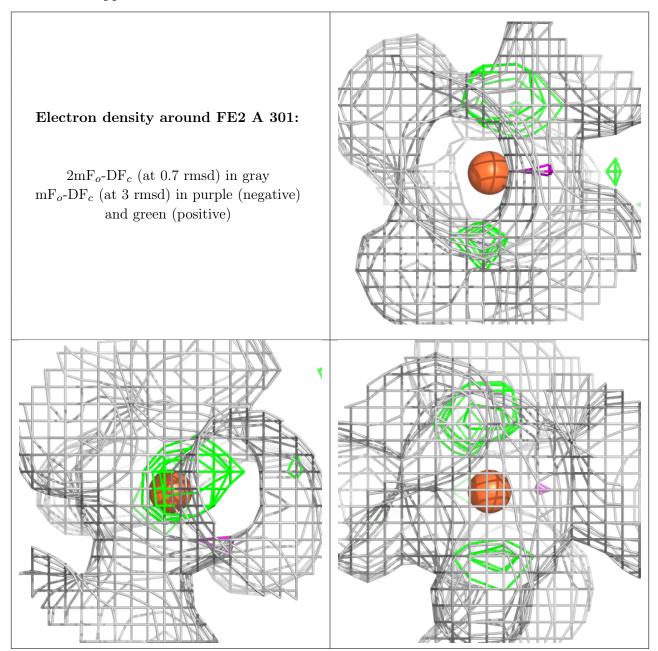
6.4 Ligands (i)

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, 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.

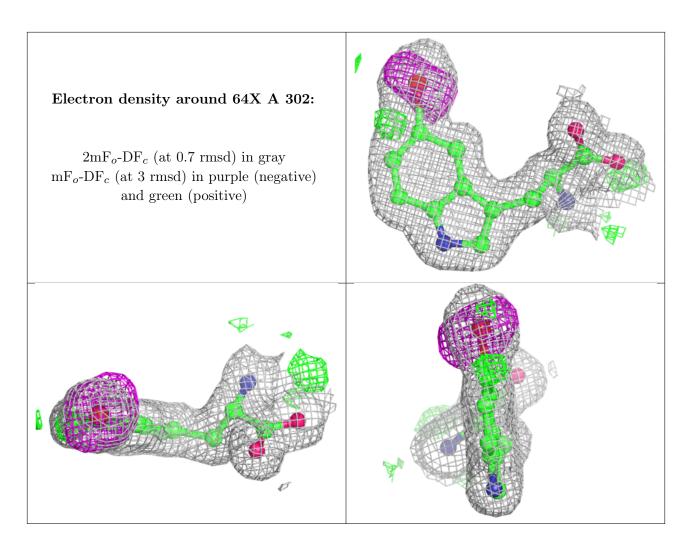
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
5	TRS	А	307	8/8	0.75	0.31	$36,\!47,\!51,\!57$	0
5	TRS	А	306	8/8	0.93	0.10	28,33,35,35	0
4	NI	В	304	1/1	0.95	0.04	44,44,44,44	0
4	NI	А	304	1/1	0.97	0.14	48,48,48,48	0
4	NI	А	305	1/1	0.98	0.06	$38,\!38,\!38,\!38$	0
4	NI	А	303	1/1	0.98	0.03	31,31,31,31	0
4	NI	В	303	1/1	0.99	0.11	53,53,53,53	0
2	FE2	А	301	1/1	0.99	0.10	20,20,20,20	0
3	64X	А	302	16/16	0.99	0.12	20,21,25,27	0
3	64X	В	302	16/16	0.99	0.12	21,23,28,28	0
2	FE2	В	301	1/1	1.00	0.08	22,22,22,22	0



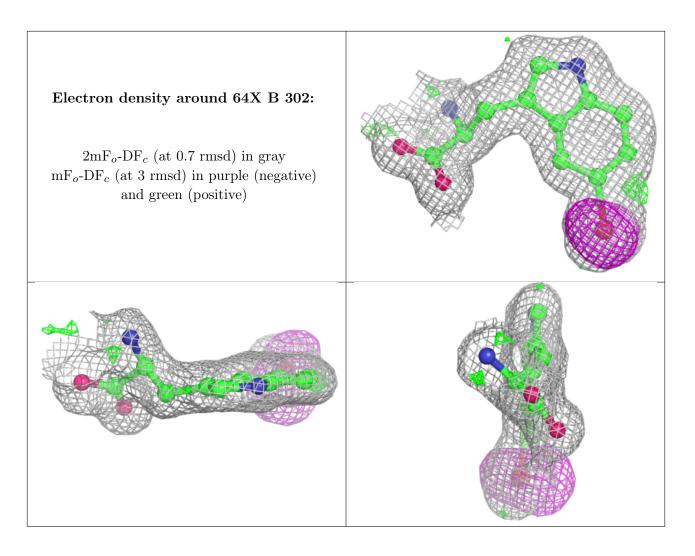
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



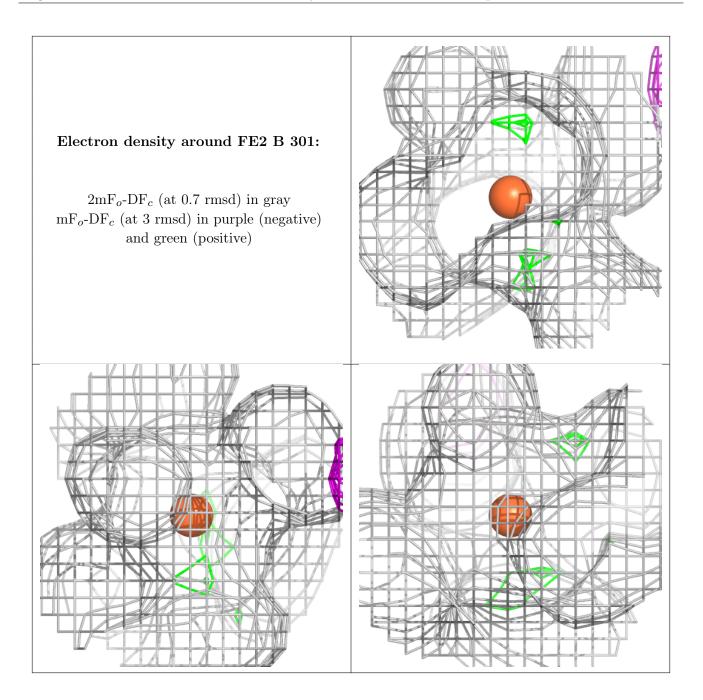












6.5 Other polymers (i)

There are no such residues in this entry.

