



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:25 am BST

PDB ID : 6AZW
Title : IDO1/FXB-001116 crystal structure
Authors : Lewis, H.A.; Lammens, A.; Steinbacher, S.
Deposited on : 2017-09-13
Resolution : 2.78 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

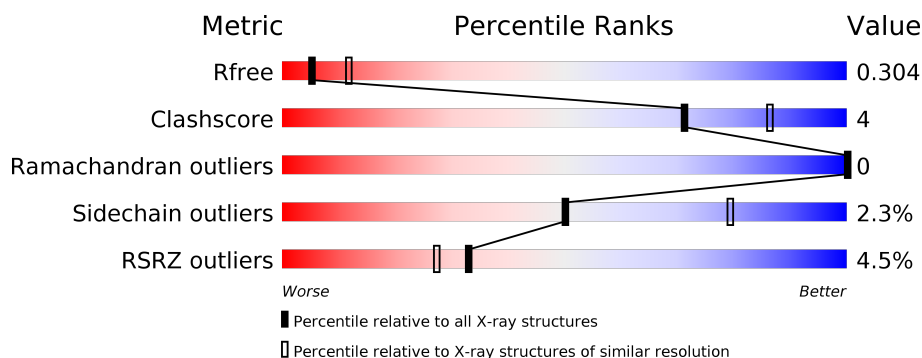
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 $\leq 5\%$. 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	394	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• 5%</div> </div> </div>
1	B	394	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• 5%</div> </div> </div>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11213 atoms, of which 5500 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.

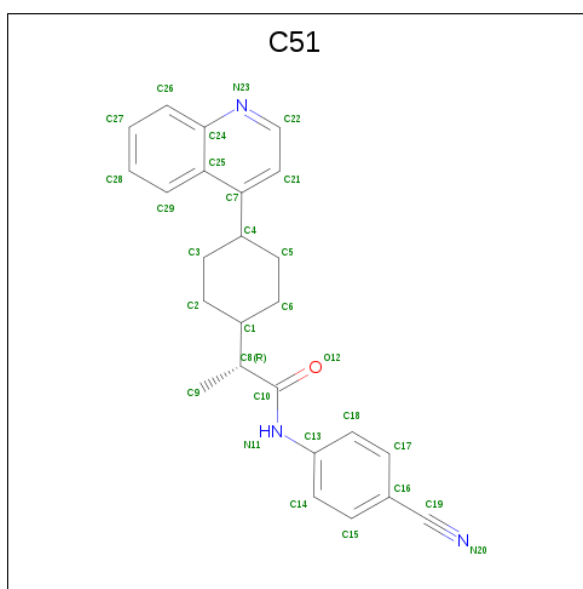
- Molecule 1 is a protein called Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	375	Total	C	H	N	O	S	0	0	0
			5690	1865	2817	482	510	16			
1	B	373	Total	C	H	N	O	S	0	0	0
			5415	1807	2633	463	496	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	MET	-	initiating methionine	UNP P14902
B	10	MET	-	initiating methionine	UNP P14902

- Molecule 2 is (2R)-N-(4-cyanophenyl)-2-[cis-4-(quinolin-4-yl)cyclohexyl]propanamide (three-letter code: C51) (formula: C₂₅H₂₅N₃O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			54	25	25	3	1		

Continued on next page...

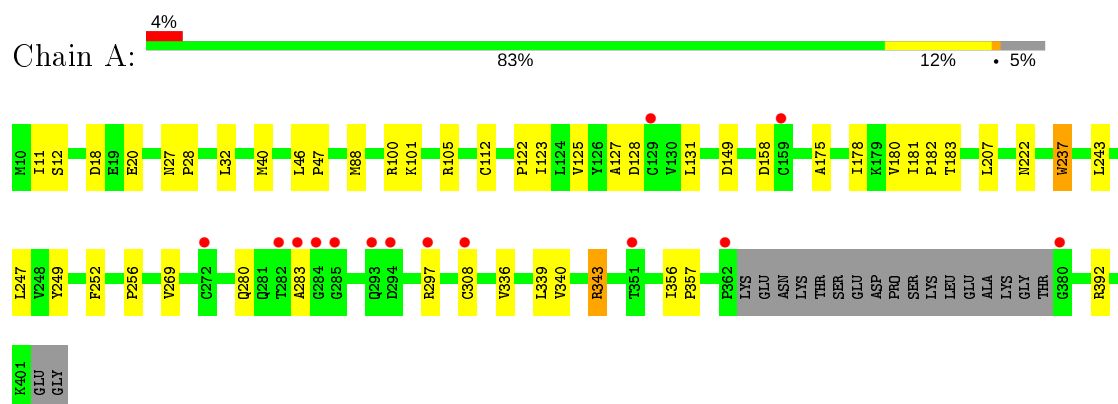
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	0	0
			54	25	25	3	1		

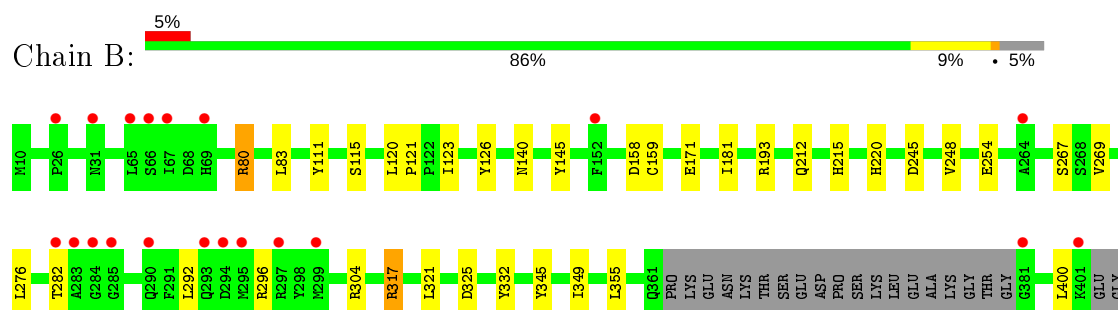
3 Residue-property plots [i](#)

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: Indoleamine 2,3-dioxygenase 1



- Molecule 1: Indoleamine 2,3-dioxygenase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.21 Å 92.56 Å 128.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.28 – 2.78 46.28 – 2.78	Depositor EDS
% Data completeness (in resolution range)	95.9 (46.28-2.78) 96.0 (46.28-2.78)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.77 Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.217 , 0.299 0.219 , 0.304	Depositor DCC
R_{free} test set	740 reflections (2.93%)	wwPDB-VP
Wilson B-factor (Å ²)	70.3	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11213	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C51

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	0.81	1/2941 (0.0%)	0.85	2/3994 (0.1%)
1	B	0.76	3/2848 (0.1%)	0.79	2/3883 (0.1%)
All	All	0.78	4/5789 (0.1%)	0.82	4/7877 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	PRO	C-N	7.39	1.48	1.34
1	A	308	CYS	CB-SG	-7.10	1.70	1.82
1	B	267	SER	CB-OG	6.37	1.50	1.42
1	B	254	GLU	C-N	-5.47	1.21	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	105	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	317	ARG	CA-CB-CG	5.69	125.93	113.40
1	B	245	ASP	CB-CG-OD1	-5.04	113.77	118.30

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	2873	2817	2795	24	0
1	B	2782	2633	2631	15	0
2	A	29	25	0	0	0
2	B	29	25	0	0	0
All	All	5713	5500	5426	39	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.

All (39) 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:123:ILE:HD12	1:A:237:TRP:CZ2	2.38	0.58
1:A:125:VAL:O	1:A:128:ASP:HB2	2.03	0.57
1:B:126:TYR:OH	1:B:171:GLU:OE1	2.18	0.56
1:B:80:ARG:NH2	1:B:123:ILE:O	2.38	0.55
1:A:343:ARG:HD2	1:A:343:ARG:N	2.22	0.54
1:B:193:ARG:NE	1:B:325:ASP:OD2	2.35	0.54
1:A:181:ILE:N	1:A:182:PRO:HD2	2.25	0.52
1:B:292:LEU:O	1:B:296:ARG:HG3	2.11	0.51
1:A:356:ILE:HB	1:A:357:PRO:HD3	1.94	0.49
1:A:27:ASN:N	1:A:28:PRO:HD3	2.27	0.49
1:B:115:SER:HB3	1:B:120:LEU:O	2.11	0.49
1:B:145:TYR:CE2	1:B:220:HIS:CD2	3.02	0.48
1:B:158:ASP:N	1:B:158:ASP:OD1	2.43	0.47
1:B:158:ASP:O	1:B:159:CYS:HB2	2.15	0.47
1:B:212:GLN:O	1:B:215:HIS:HB2	2.15	0.47
1:A:207:LEU:HD13	1:A:339:LEU:HD23	1.98	0.46
1:B:181:ILE:HG12	1:B:276:LEU:HD22	1.98	0.45
1:A:46:LEU:HB2	1:A:47:PRO:HD3	1.99	0.45
1:A:336:VAL:O	1:A:340:VAL:HG23	2.17	0.45
1:A:32:LEU:H	1:A:40:MET:CE	2.30	0.44
1:A:180:VAL:O	1:A:183:THR:N	2.47	0.44
1:A:175:ALA:HA	1:A:178:ILE:HD12	1.99	0.44
1:B:345:TYR:CE2	1:B:349:ILE:HD11	2.52	0.44
1:A:88:MET:HE1	1:A:123:ILE:HD11	2.00	0.44
1:B:83:LEU:HD13	1:B:111:TYR:HA	2.00	0.43
1:B:321:LEU:HD21	1:B:400:LEU:HD22	2.01	0.43
1:A:247:LEU:O	1:A:256:PRO:HA	2.19	0.43
1:A:280:GLN:HB3	1:A:283:ALA:HB3	2.00	0.42
1:A:11:ILE:HG22	1:A:12:SER:N	2.34	0.42
1:A:123:ILE:HD12	1:A:237:TRP:CE2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:CYS:HB3	1:A:252:PHE:CD2	2.54	0.42
1:A:247:LEU:HD23	1:A:249:TYR:CZ	2.55	0.42
1:A:122:PRO:HB2	1:A:249:TYR:CE2	2.55	0.41
1:A:101:LYS:HG2	1:A:243:LEU:CD2	2.50	0.41
1:B:317:ARG:HD3	1:B:332:TYR:OH	2.21	0.41
1:A:127:ALA:HA	1:A:131:LEU:HD12	2.02	0.41
1:A:18:ASP:OD2	1:A:20:GLU:HB3	2.21	0.41
1:A:158:ASP:OD1	1:A:158:ASP:N	2.53	0.40
1:B:140:ASN:O	1:B:140:ASN:ND2	2.55	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	371/394 (94%)	361 (97%)	10 (3%)	0	100	100
1	B	369/394 (94%)	357 (97%)	12 (3%)	0	100	100
All	All	740/788 (94%)	718 (97%)	22 (3%)	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	289/341 (85%)	282 (98%)	7 (2%)	49	78
1	B	268/341 (79%)	262 (98%)	6 (2%)	52	80
All	All	557/682 (82%)	544 (98%)	13 (2%)	50	79

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ASP
1	A	222	ASN
1	A	237	TRP
1	A	269	VAL
1	A	297	ARG
1	A	343	ARG
1	A	392	ARG
1	B	80	ARG
1	B	248	VAL
1	B	269	VAL
1	B	282	THR
1	B	304	ARG
1	B	355	LEU

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

Mol	Chain	Res	Type
1	A	191	GLN
1	A	305	ASN
1	A	386	ASN
1	B	76	GLN
1	B	140	ASN
1	B	191	GLN
1	B	360	GLN
1	B	386	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 carbohydrates in this entry.

5.6 Ligand geometry

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	C51	A	501	-	32,32,32	0.53	0	44,44,44	0.53	0
2	C51	B	501	-	32,32,32	0.48	0	44,44,44	0.49	0

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	C51	A	501	-	-	1/18/28/28	0/4/4/4
2	C51	B	501	-	-	2/18/28/28	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

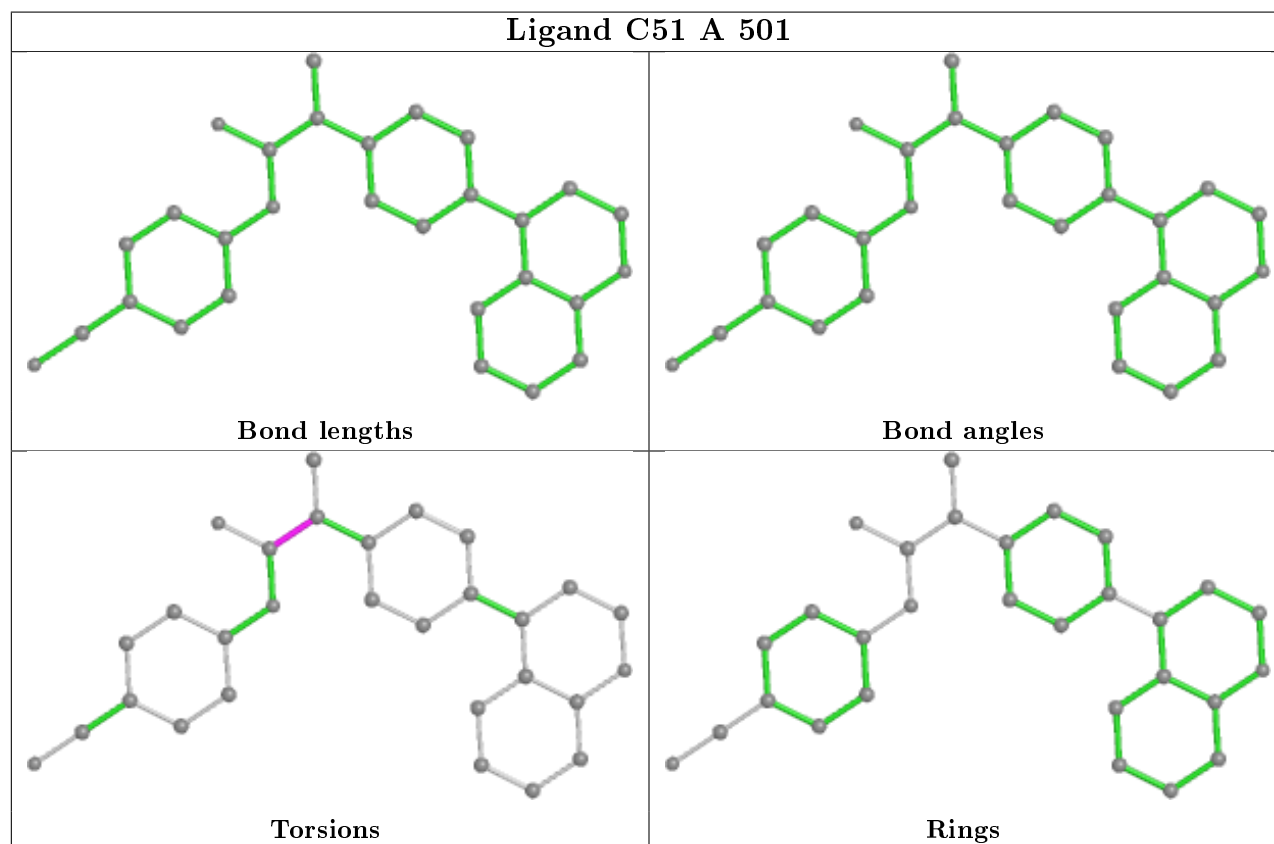
All (3) torsion outliers are listed below:

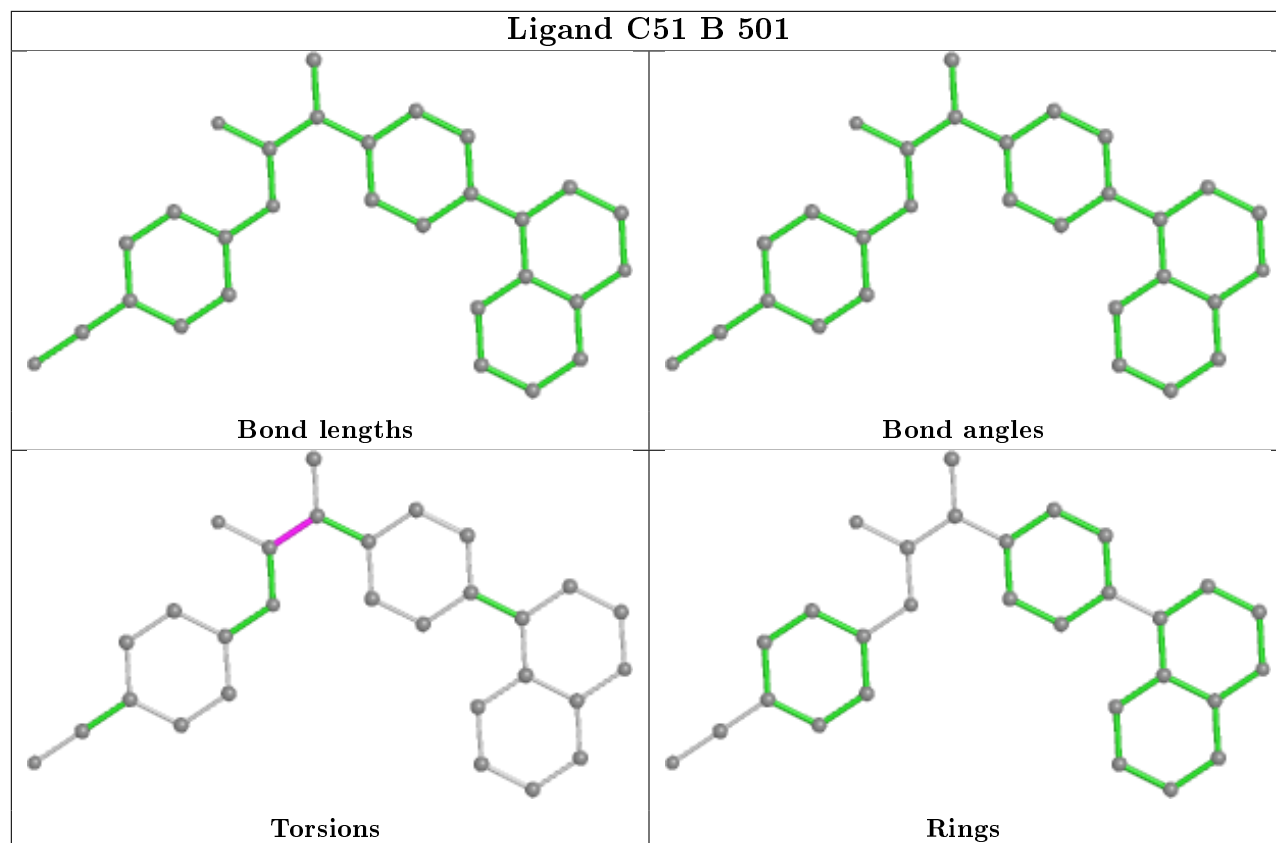
Mol	Chain	Res	Type	Atoms
2	B	501	C51	N11-C10-C8-C1
2	B	501	C51	O12-C10-C8-C1
2	A	501	C51	N11-C10-C8-C1

There are no ring outliers.

No monomer is involved in short contacts.

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 [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, 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	375/394 (95%)	0.03	14 (3%) 41 36	43, 82, 133, 273	0
1	B	373/394 (94%)	0.20	20 (5%) 25 20	55, 90, 147, 294	0
All	All	748/788 (94%)	0.12	34 (4%) 33 27	43, 86, 140, 294	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	295	MET	6.3
1	A	129	CYS	4.4
1	A	282	THR	3.7
1	B	283	ALA	3.5
1	B	381	GLY	3.5
1	B	69	HIS	3.3
1	A	159	CYS	3.2
1	B	282	THR	3.1
1	B	294	ASP	3.1
1	B	65	LEU	3.0
1	A	283	ALA	2.9
1	B	284	GLY	2.8
1	B	66	SER	2.7
1	A	380	GLY	2.7
1	A	272	CYS	2.6
1	B	299	MET	2.6
1	B	26	PRO	2.5
1	B	290	GLN	2.5
1	A	293	GLN	2.4
1	A	284	GLY	2.4
1	A	285	GLY	2.4
1	A	351	THR	2.4
1	B	264	ALA	2.3
1	B	31	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	285	GLY	2.2
1	A	294	ASP	2.1
1	B	401	LYS	2.1
1	A	362	PRO	2.1
1	A	308	CYS	2.1
1	B	152	PHE	2.1
1	B	293	GLN	2.0
1	B	67	ILE	2.0
1	A	297	ARG	2.0
1	B	297	ARG	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 carbohydrates in this entry.

6.4 Ligands [i](#)

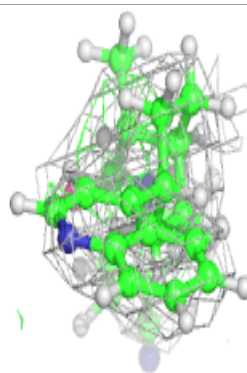
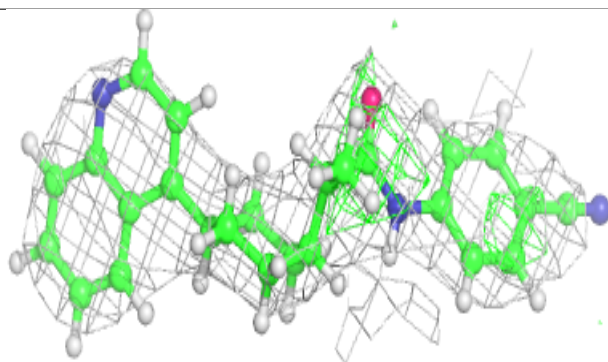
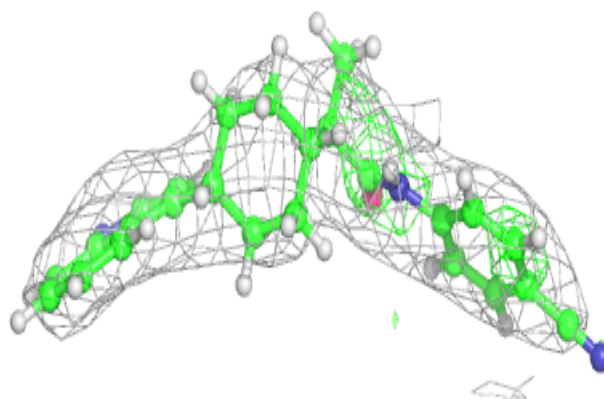
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	C51	B	501	29/29	0.91	0.41	102,128,170,176	0
2	C51	A	501	29/29	0.94	0.22	47,85,132,137	0

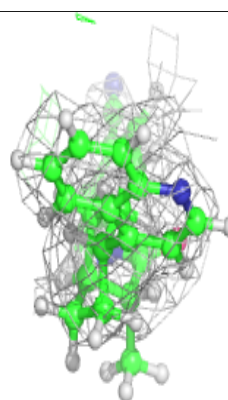
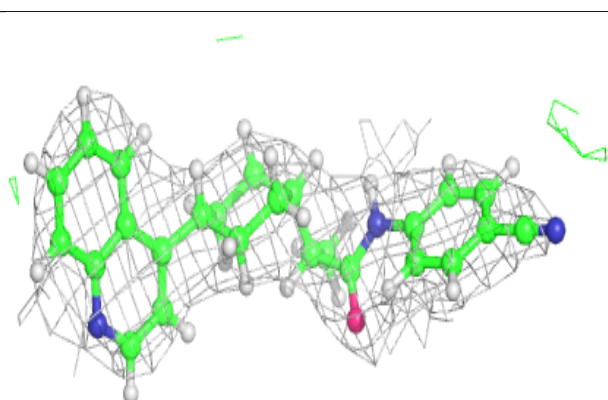
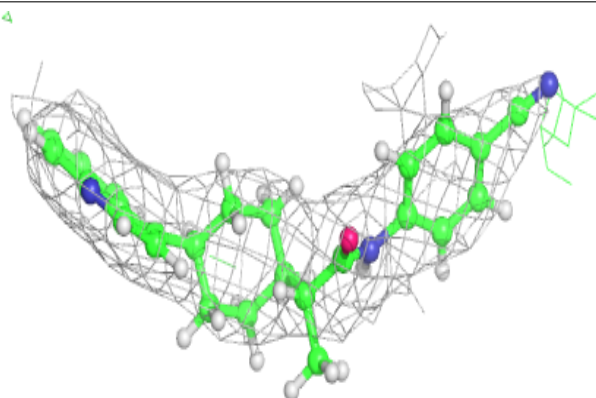
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C51 B 501:

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

**Electron density around C51 A 501:**

$2mF_o-DF_c$ (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.