



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 12:07 pm GMT

PDB ID : 8QV7  
Title : Crystal structure of human TDO with alpha-methyl-L-tryptophan  
Authors : Wicki, M.; Mac Sweeney, A.  
Deposited on : 2023-10-17  
Resolution : 2.93 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

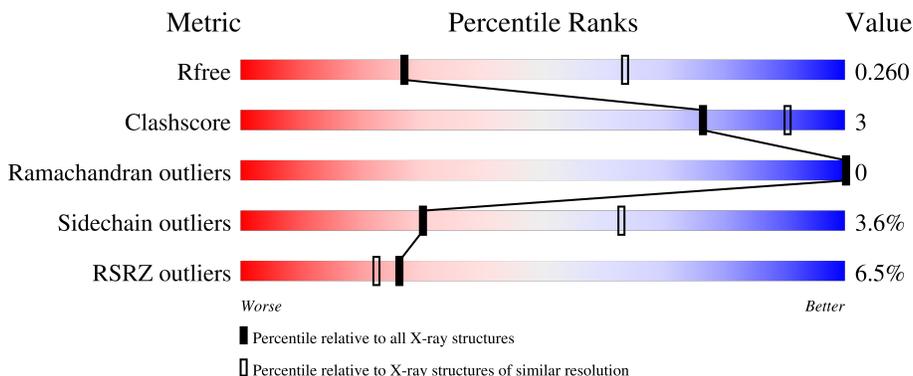
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.93 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))
$R_{free}$	164625	2797 (2.94-2.90)
Clashscore	180529	3049 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (2.94-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	355	
1	B	355	
1	C	355	
1	D	355	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 10018 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.

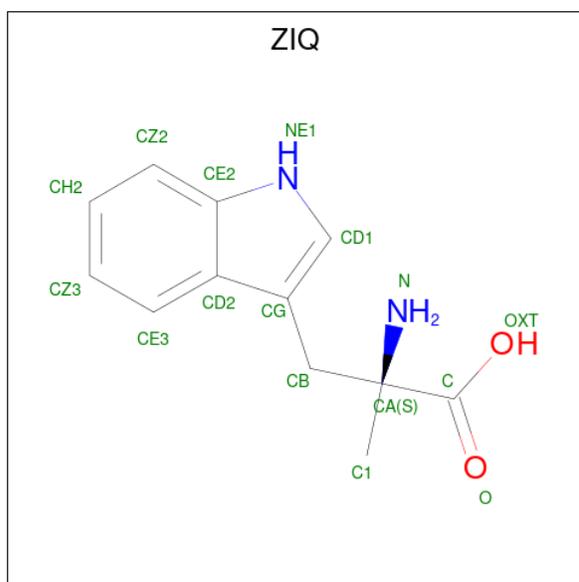
- Molecule 1 is a protein called Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	318	2526	1639	430	447	10	0	0	0
1	B	310	2472	1607	426	429	10	0	1	0
1	C	305	2420	1576	409	426	9	0	0	0
1	D	313	2512	1632	427	443	10	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

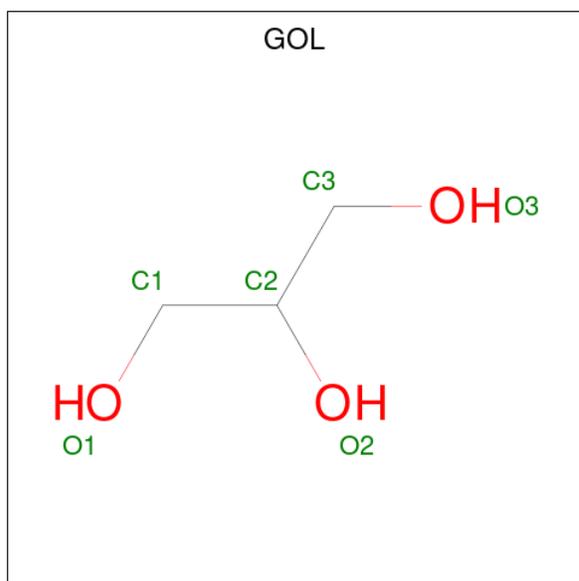
Chain	Residue	Modelled	Actual	Comment	Reference
A	390	GLU	-	expression tag	UNP P48775
A	391	HIS	-	expression tag	UNP P48775
A	392	HIS	-	expression tag	UNP P48775
A	393	HIS	-	expression tag	UNP P48775
B	390	GLU	-	expression tag	UNP P48775
B	391	HIS	-	expression tag	UNP P48775
B	392	HIS	-	expression tag	UNP P48775
B	393	HIS	-	expression tag	UNP P48775
C	390	GLU	-	expression tag	UNP P48775
C	391	HIS	-	expression tag	UNP P48775
C	392	HIS	-	expression tag	UNP P48775
C	393	HIS	-	expression tag	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391	HIS	-	expression tag	UNP P48775
D	392	HIS	-	expression tag	UNP P48775
D	393	HIS	-	expression tag	UNP P48775

- Molecule 2 is alpha-methyl-L-tryptophan (three-letter code: ZIQ) (formula: C<sub>12</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			
2	A	1	Total	16	12	2	2	0	0
2	B	1	Total	16	12	2	2	0	0
2	C	1	Total	16	12	2	2	0	0
2	D	1	Total	16	12	2	2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

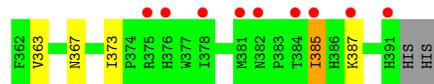


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

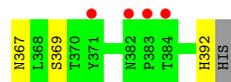
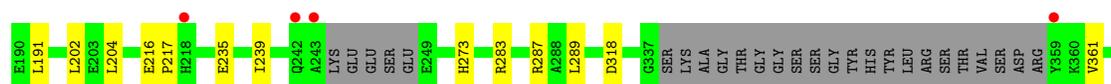
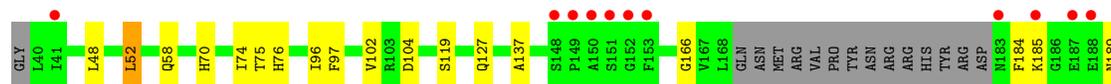
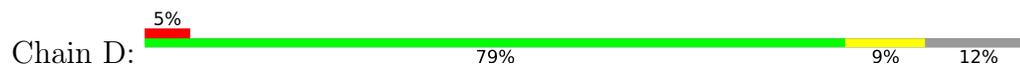
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	5	Total	O	0	0
			5	5		
4	C	2	Total	O	0	0
			2	2		
4	D	2	Total	O	0	0
			2	2		





● Molecule 1: Tryptophan 2,3-dioxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.28Å 90.76Å 132.77Å 90.00° 120.75° 90.00°	Depositor
Resolution (Å)	41.35 – 2.93 41.35 – 2.93	Depositor EDS
% Data completeness (in resolution range)	94.1 (41.35-2.93) 77.3 (41.35-2.93)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.65Å)	Xtrriage
Refinement program	BUSTER 2.11.8	Depositor
R, $R_{free}$	0.246 , 0.273 0.231 , 0.260	Depositor DCC
$R_{free}$ test set	10649 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtrriage
Anisotropy	0.075	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	10018	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZIQ, GOL

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	0.35	0/2584	0.51	0/3500
1	B	0.35	0/2533	0.50	0/3428
1	C	0.35	0/2473	0.51	0/3347
1	D	0.35	0/2570	0.51	0/3477
All	All	0.35	0/10160	0.51	0/13752

There are no bond length outliers.

There are no bond angle outliers.

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	2526	0	2372	16	0
1	B	2472	0	2346	13	0
1	C	2420	0	2279	16	0
1	D	2512	0	2375	14	0
2	A	16	0	0	0	0
2	B	16	0	0	0	0
2	C	16	0	0	1	0
2	D	16	0	0	0	0
3	A	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
4	A	3	0	0	0	0
4	B	5	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
All	All	10018	0	9388	55	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 3.

All (55) 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:334:ARG:HE	1:A:335:MET:CE	1.97	0.76
1:A:334:ARG:HE	1:A:335:MET:HE1	1.58	0.67
3:A:402:GOL:H12	1:C:323:LYS:HD3	1.75	0.67
1:B:273:HIS:CE1	1:B:289:LEU:HD13	2.38	0.59
1:A:334:ARG:HE	1:A:335:MET:HE2	1.68	0.58
1:A:273:HIS:CE1	1:A:289:LEU:HD13	2.39	0.57
1:C:273:HIS:CE1	1:C:289:LEU:HD13	2.39	0.57
1:D:273:HIS:CE1	1:D:289:LEU:HD13	2.40	0.57
1:A:70:HIS:CE1	1:A:74:ILE:HD13	2.40	0.56
1:D:48:LEU:HB3	1:D:52:LEU:HD22	1.88	0.56
1:A:240:ARG:HH22	1:A:253:GLN:NE2	2.04	0.56
1:B:70:HIS:CE1	1:B:74:ILE:HD13	2.41	0.55
1:C:70:HIS:CE1	1:C:74:ILE:HD13	2.40	0.55
1:B:303:ARG:NH2	1:B:391:HIS:CD2	2.75	0.55
1:D:166:GLY:O	1:D:283:ARG:NH1	2.40	0.55
1:A:360:LYS:HB2	1:A:363:VAL:HG13	1.87	0.54
1:B:137:ALA:HB3	1:D:369:SER:HB3	1.89	0.54
1:C:46:LEU:HD21	1:D:76:HIS:HB3	1.89	0.54
1:A:166:GLY:O	1:A:283:ARG:NH1	2.42	0.53
1:C:166:GLY:O	1:C:283:ARG:NH1	2.42	0.52
1:C:96:ILE:HG22	1:C:102:VAL:HG13	1.92	0.52
1:D:70:HIS:CE1	1:D:74:ILE:HD13	2.46	0.51
1:B:166:GLY:O	1:B:283:ARG:NH1	2.43	0.51
1:D:96:ILE:HG22	1:D:102:VAL:HG13	1.93	0.51
1:C:185:LYS:HA	1:C:189:ASN:HB2	1.94	0.50
1:C:202:LEU:HD13	1:C:361:VAL:HG12	1.95	0.49
1:B:96:ILE:HG22	1:B:102:VAL:HG13	1.95	0.49
1:A:235:GLU:O	1:A:239:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ASP:HA	1:D:392:HIS:HA	1.96	0.47
1:D:185:LYS:HA	1:D:189:ASN:HB2	1.97	0.47
1:B:385:ILE:HA	1:B:388[B]:PHE:CE1	2.50	0.47
1:C:235:GLU:O	1:C:239:ILE:HG12	2.16	0.46
1:D:202:LEU:HD13	1:D:361:VAL:HG12	1.97	0.46
1:C:95:GLU:O	1:C:99:ASN:HB2	2.16	0.45
1:B:185:LYS:HA	1:B:189:ASN:HB2	1.98	0.45
1:B:202:LEU:HD13	1:B:361:VAL:HG12	1.98	0.45
1:A:202:LEU:HD13	1:A:361:VAL:HG12	1.98	0.44
1:A:385:ILE:HG22	1:A:387:LYS:CG	2.48	0.44
1:D:216:GLU:HA	1:D:217:PRO:HD3	1.92	0.44
1:C:385:ILE:HG22	1:C:387:LYS:HG3	1.98	0.44
1:C:385:ILE:HG22	1:C:387:LYS:CG	2.48	0.43
1:A:70:HIS:CE1	1:A:74:ILE:CD1	3.02	0.43
1:A:84:LYS:HD2	1:B:52:LEU:HD22	1.99	0.43
1:D:97:PHE:HB3	1:D:204:LEU:HB3	2.01	0.43
1:B:369:SER:HB3	1:D:137:ALA:HB3	2.00	0.43
1:C:216:GLU:HA	1:C:217:PRO:HD3	1.91	0.43
1:B:235:GLU:O	1:B:239:ILE:HG12	2.19	0.43
1:C:70:HIS:CE1	1:C:74:ILE:CD1	3.03	0.42
1:C:264:LEU:HD22	1:C:373:ILE:HD11	2.02	0.41
1:A:240:ARG:HH22	1:A:253:GLN:HE21	1.67	0.41
2:C:401:ZIQ:CD1	2:C:401:ZIQ:C	2.98	0.41
1:D:235:GLU:O	1:D:239:ILE:HG13	2.21	0.41
1:C:97:PHE:HB3	1:C:204:LEU:HB3	2.02	0.40
1:A:97:PHE:HB3	1:A:204:LEU:HB3	2.02	0.40
1:A:124:LEU:HD22	1:B:131:ILE:CD1	2.51	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	312/355 (88%)	303 (97%)	9 (3%)	0	100	100
1	B	303/355 (85%)	297 (98%)	6 (2%)	0	100	100
1	C	295/355 (83%)	287 (97%)	8 (3%)	0	100	100
1	D	305/355 (86%)	298 (98%)	7 (2%)	0	100	100
All	All	1215/1420 (86%)	1185 (98%)	30 (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	249/327 (76%)	238 (96%)	11 (4%)	24	55
1	B	247/327 (76%)	240 (97%)	7 (3%)	38	71
1	C	238/327 (73%)	231 (97%)	7 (3%)	37	70
1	D	251/327 (77%)	241 (96%)	10 (4%)	27	59
All	All	985/1308 (75%)	950 (96%)	35 (4%)	30	63

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	74	ILE
1	A	119	SER
1	A	127	GLN
1	A	191	LEU
1	A	314	LEU
1	A	318	ASP
1	A	363	VAL
1	A	367	ASN
1	A	381	MET
1	A	385	ILE
1	B	58	GLN
1	B	75	THR

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Mol	Chain	Res	Type
1	B	127	GLN
1	B	191	LEU
1	B	216	GLU
1	B	318	ASP
1	B	367	ASN
1	C	58	GLN
1	C	127	GLN
1	C	191	LEU
1	C	318	ASP
1	C	363	VAL
1	C	367	ASN
1	C	385	ILE
1	D	52	LEU
1	D	58	GLN
1	D	75	THR
1	D	119	SER
1	D	127	GLN
1	D	184	PHE
1	D	191	LEU
1	D	287	ARG
1	D	318	ASP
1	D	367	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	253	GLN
1	A	327	ASN
1	B	64	ASN
1	B	141	ASN
1	B	391	HIS
1	C	327	ASN
1	D	127	GLN
1	D	141	ASN
1	D	327	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 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
3	GOL	B	402	-	5,5,5	0.31	0	5,5,5	0.21	0
2	ZIQ	D	401	-	13,17,17	1.09	0	14,25,25	1.08	2 (14%)
2	ZIQ	B	401	-	13,17,17	1.16	0	14,25,25	1.10	2 (14%)
3	GOL	A	402	-	5,5,5	0.23	0	5,5,5	0.05	0
2	ZIQ	C	401	-	13,17,17	1.19	0	14,25,25	1.08	2 (14%)
2	ZIQ	A	401	-	13,17,17	1.13	0	14,25,25	1.05	2 (14%)

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
3	GOL	B	402	-	-	0/4/4/4	-
2	ZIQ	D	401	-	-	0/9/11/11	0/2/2/2
2	ZIQ	B	401	-	-	2/9/11/11	0/2/2/2
3	GOL	A	402	-	-	2/4/4/4	-
2	ZIQ	C	401	-	-	4/9/11/11	0/2/2/2
2	ZIQ	A	401	-	-	0/9/11/11	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	ZIQ	CE3-CD2-CE2	2.58	121.59	118.17
2	A	401	ZIQ	CE3-CD2-CG	-2.54	129.76	134.42
2	C	401	ZIQ	CE3-CD2-CE2	2.51	121.49	118.17
2	D	401	ZIQ	CE3-CD2-CE2	2.49	121.47	118.17
2	B	401	ZIQ	CE3-CD2-CG	-2.46	129.89	134.42
2	C	401	ZIQ	CE3-CD2-CG	-2.43	129.95	134.42
2	D	401	ZIQ	CE3-CD2-CG	-2.36	130.08	134.42
2	A	401	ZIQ	CE3-CD2-CE2	2.36	121.29	118.17

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	ZIQ	O-C-CA-C1
2	C	401	ZIQ	OXT-C-CA-C1
3	A	402	GOL	C1-C2-C3-O3
3	A	402	GOL	O2-C2-C3-O3
2	C	401	ZIQ	O-C-CA-CB
2	C	401	ZIQ	OXT-C-CA-CB
2	B	401	ZIQ	O-C-CA-CB
2	B	401	ZIQ	OXT-C-CA-CB

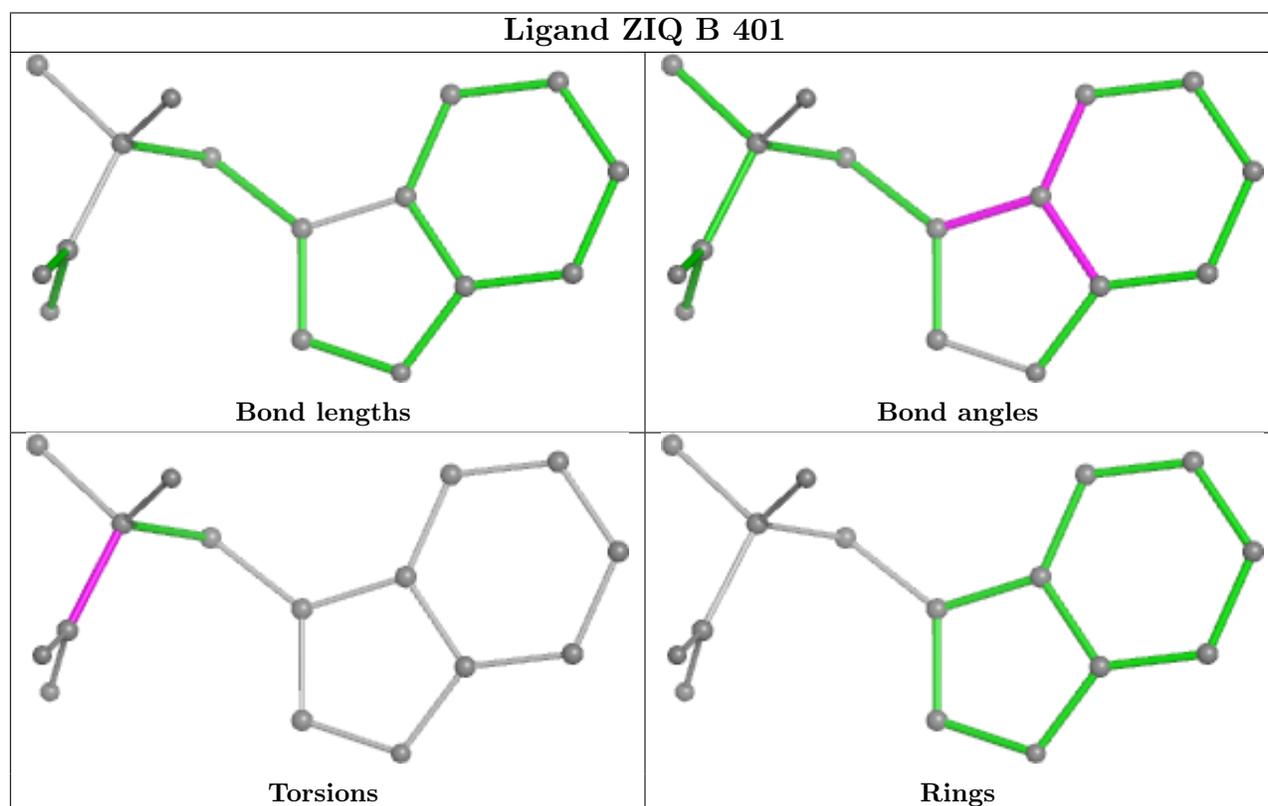
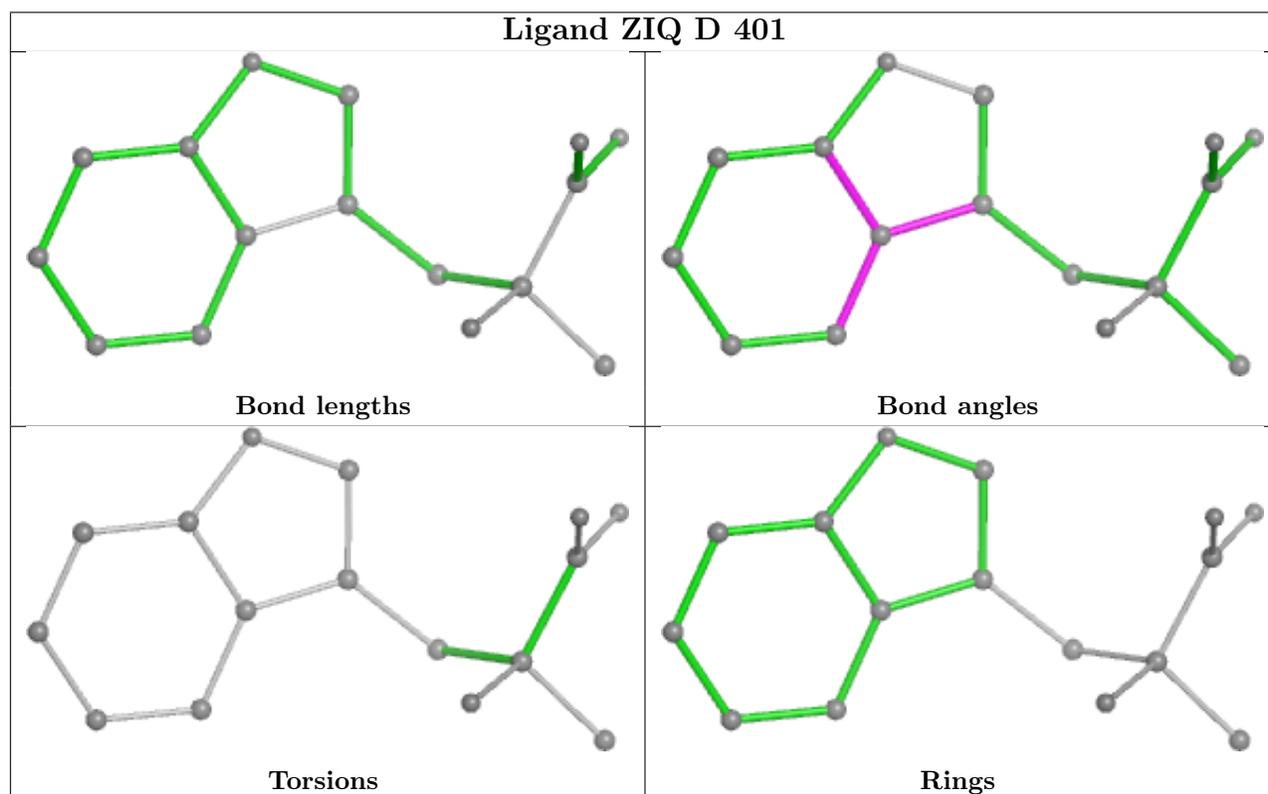
There are no ring outliers.

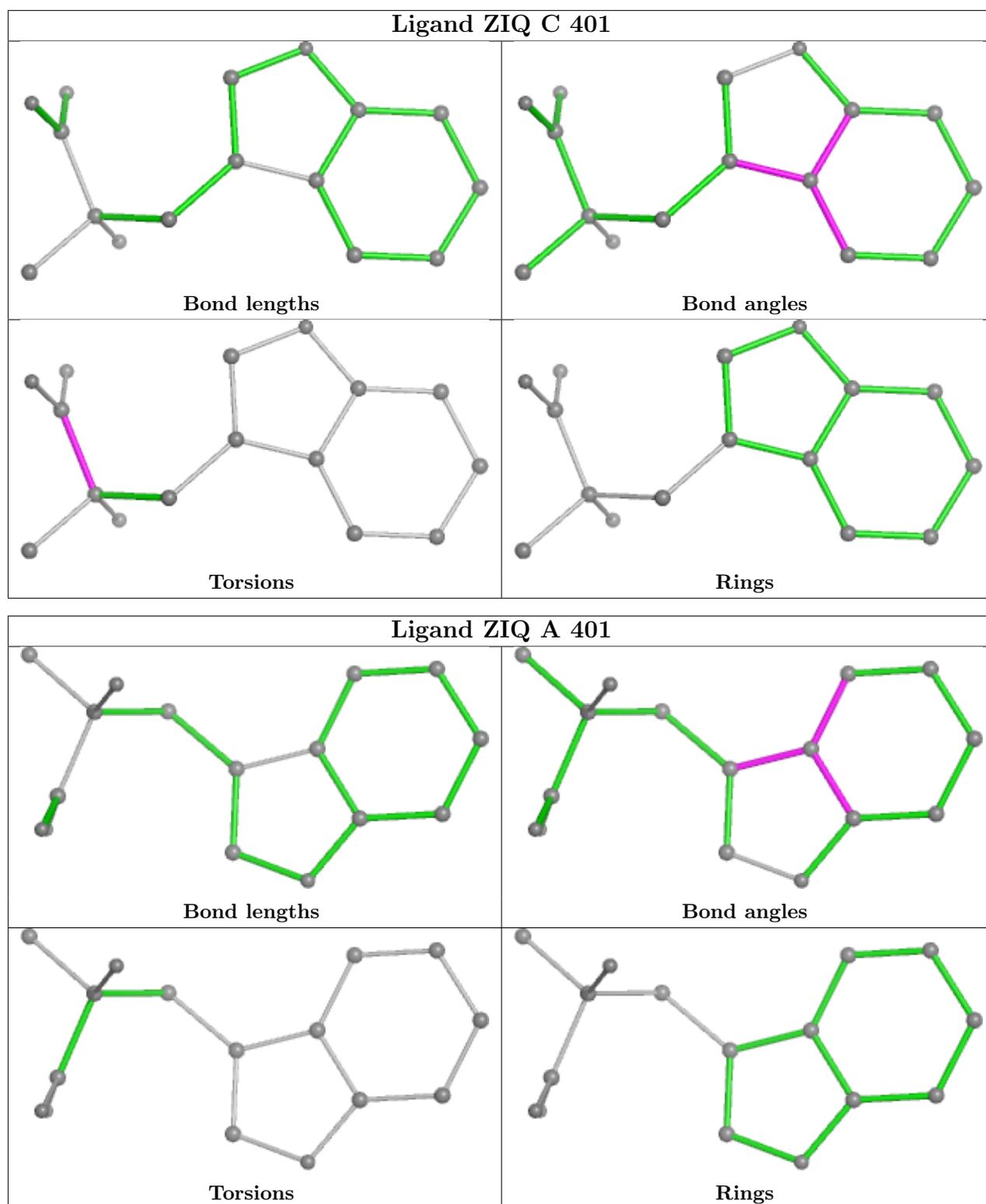
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	GOL	1	0
2	C	401	ZIQ	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 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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	318/355 (89%)	0.56	23 (7%) 23 20	34, 57, 77, 91	0
1	B	310/355 (87%)	0.43	20 (6%) 26 22	31, 50, 79, 96	1 (0%)
1	C	305/355 (85%)	0.57	19 (6%) 28 24	32, 56, 73, 86	0
1	D	313/355 (88%)	0.34	19 (6%) 28 24	33, 50, 75, 83	0
All	All	1246/1420 (87%)	0.47	81 (6%) 26 22	31, 53, 76, 96	1 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	359	TYR	5.3
1	B	148	SER	4.9
1	A	385	ILE	4.6
1	D	148	SER	4.5
1	D	151	SER	4.1
1	A	384	THR	4.1
1	A	382	ASN	4.0
1	D	183	ASN	3.8
1	A	358	ARG	3.7
1	D	188	GLU	3.7
1	A	356	SER	3.6
1	B	151	SER	3.5
1	A	152	GLY	3.4
1	C	375	ARG	3.4
1	B	40	LEU	3.4
1	B	388[A]	PHE	3.3
1	C	387	LYS	3.3
1	C	251	GLU	3.3
1	C	382	ASN	3.2
1	C	384	THR	3.2
1	A	359	TYR	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	385	ILE	3.2
1	A	148	SER	3.2
1	A	333	HIS	3.1
1	C	330	CYS	3.1
1	B	358	ARG	3.1
1	A	150	ALA	3.0
1	B	150	ALA	2.9
1	C	358	ARG	2.9
1	D	359	TYR	2.8
1	A	187	GLU	2.8
1	A	62	LYS	2.8
1	C	154	GLN	2.8
1	B	383	PRO	2.7
1	D	383	PRO	2.7
1	A	375	ARG	2.7
1	A	151	SER	2.7
1	C	381	MET	2.6
1	B	240	ARG	2.6
1	C	243	ALA	2.6
1	B	371	TYR	2.6
1	D	187	GLU	2.5
1	C	188	GLU	2.5
1	D	371	TYR	2.5
1	B	41	ILE	2.5
1	D	41	ILE	2.5
1	A	338	SER	2.5
1	A	149	PRO	2.5
1	B	188	GLU	2.4
1	D	243	ALA	2.4
1	B	258	GLN	2.3
1	D	153	PHE	2.3
1	B	253	GLN	2.3
1	D	382	ASN	2.3
1	B	184	PHE	2.3
1	D	149	PRO	2.3
1	A	378	ILE	2.2
1	C	102	VAL	2.2
1	B	168	LEU	2.2
1	C	378	ILE	2.2
1	C	376	HIS	2.2
1	B	153	PHE	2.2
1	A	330	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	185	LYS	2.2
1	D	152	GLY	2.1
1	D	384	THR	2.1
1	C	99	ASN	2.1
1	C	391	HIS	2.1
1	D	185	LYS	2.1
1	A	251	GLU	2.1
1	A	260	GLN	2.1
1	D	242	GLN	2.1
1	D	150	ALA	2.1
1	A	190	GLU	2.1
1	B	133	GLU	2.1
1	A	370	THR	2.0
1	A	221	ASN	2.0
1	B	373	ILE	2.0
1	D	218	HIS	2.0
1	C	258	GLN	2.0
1	C	123	LYS	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<sup>th</sup> 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.

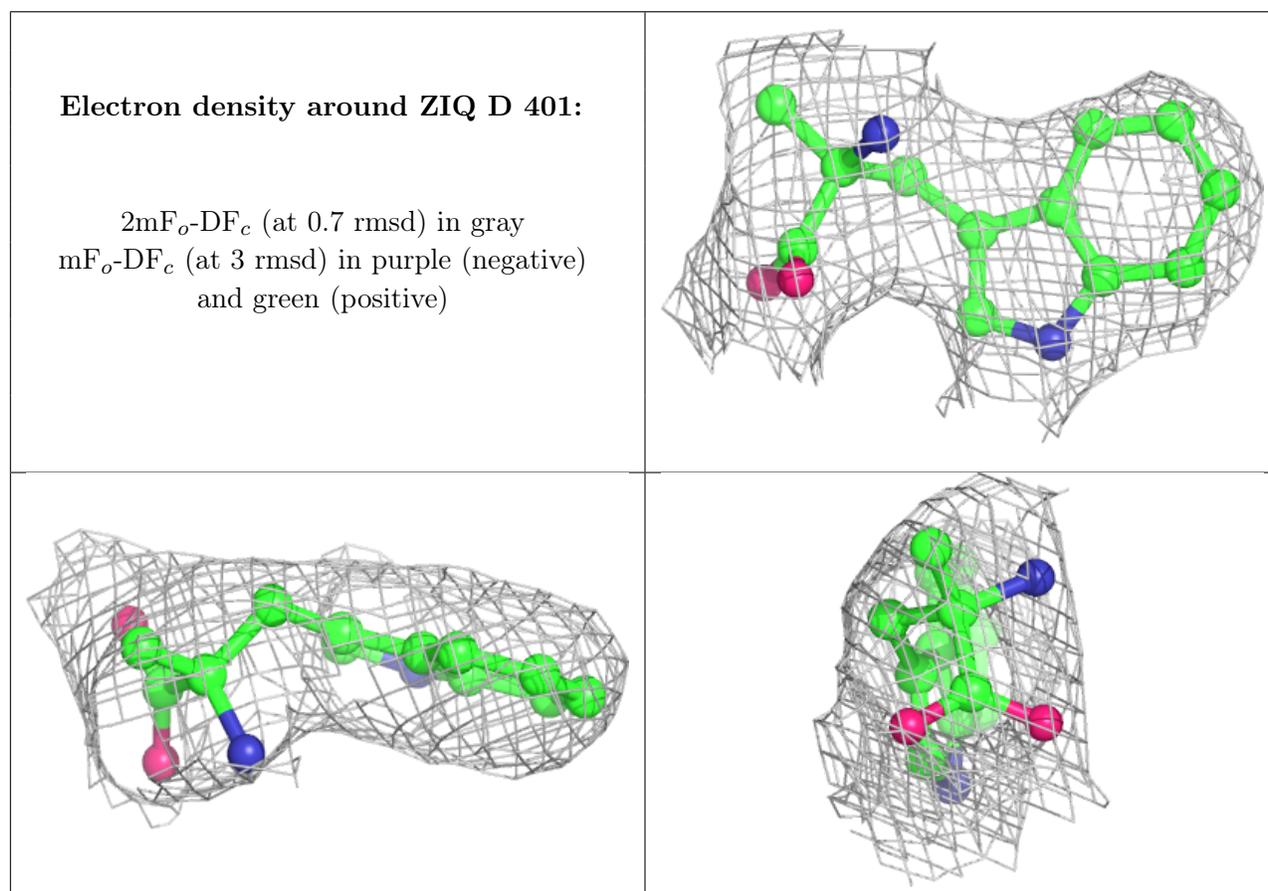
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	402	6/6	0.84	0.21	34,34,35,36	0
3	GOL	A	402	6/6	0.93	0.13	18,19,19,19	0
2	ZIQ	D	401	16/16	0.94	0.10	41,42,42,42	0
2	ZIQ	A	401	16/16	0.95	0.10	46,46,47,47	0
2	ZIQ	B	401	16/16	0.95	0.11	51,51,52,52	0

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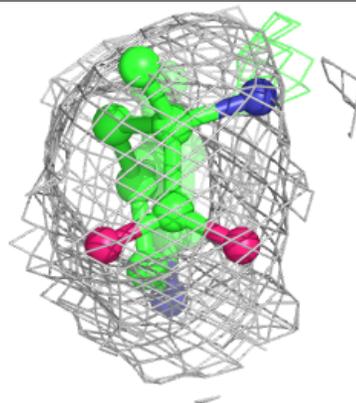
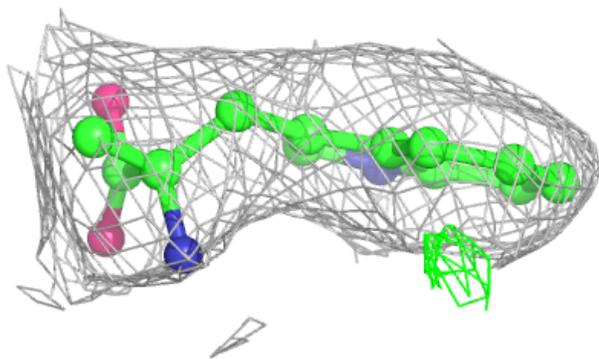
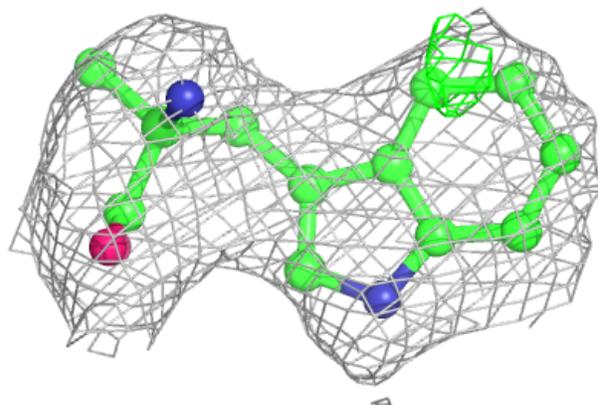
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZIQ	C	401	16/16	0.95	0.10	53,53,54,55	0

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.



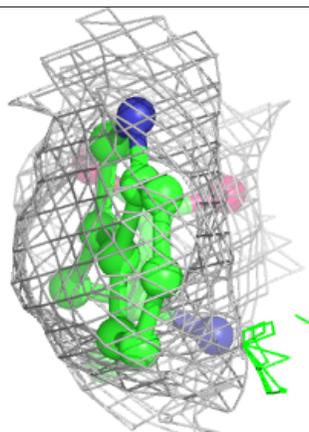
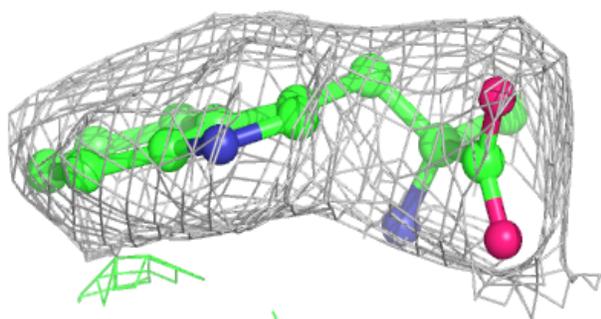
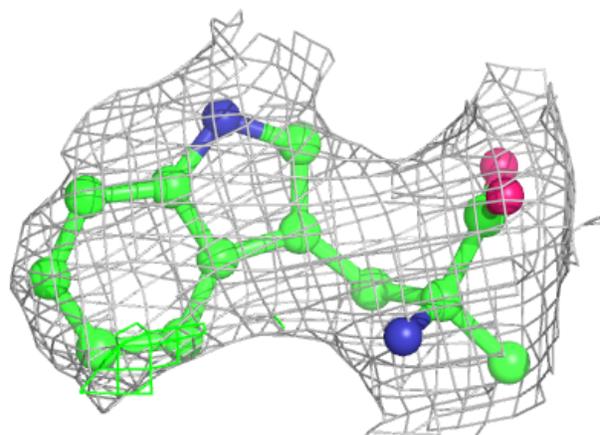
**Electron density around ZIQ A 401:**

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

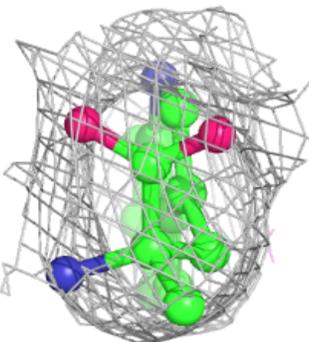
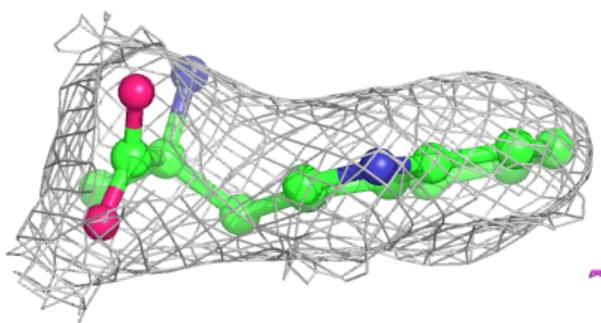
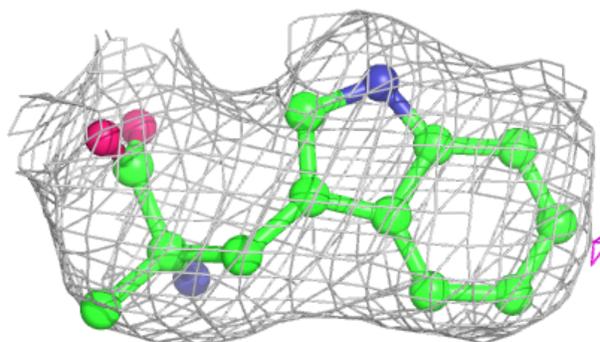


**Electron density around ZIQ B 401:**

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

**Electron density around ZIQ C 401:**

$2mF_o-DF_c$  (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.