



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:45 AM UTC

PDB ID : 8FUR / pdb_00008fur
Title : Crystal structure of human IDO1 with compound 11
Authors : Critton, D.A.; Lewis, H.A.
Deposited on : 2023-01-18
Resolution : 2.29 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

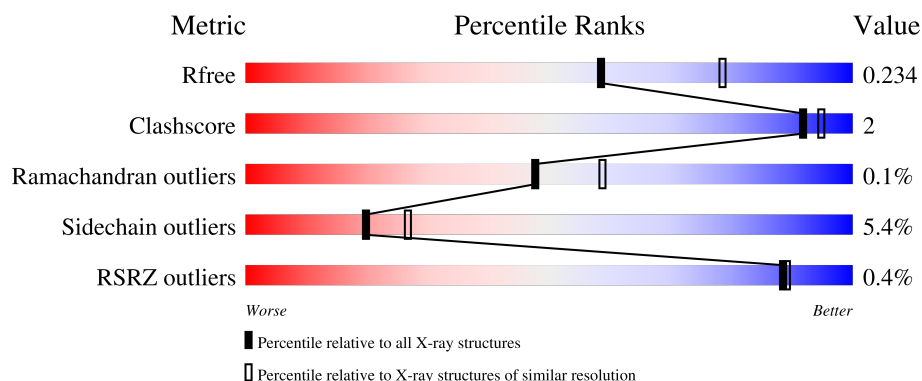
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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 $\leq 5\%$. 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	406	
1	B	406	
1	C	406	
1	D	406	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22495 atoms, of which 10914 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.

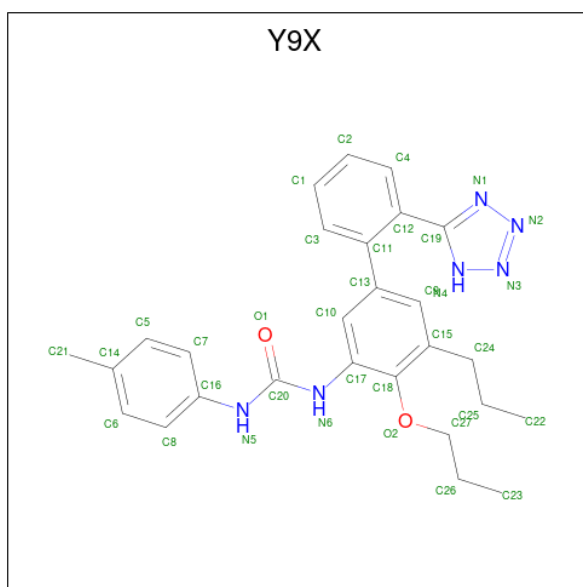
- Molecule 1 is a protein called Indoleamine 2,3-dioxygenase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	H	N	O	S	2723	0	0
			5526	1811	2723	470	505	17			
1	B	363	Total	C	H	N	O	S	2747	0	0
			5566	1823	2747	473	506	17			
1	C	353	Total	C	H	N	O	S	2669	0	0
			5411	1776	2669	458	491	17			
1	D	358	Total	C	H	N	O	S	2655	0	0
			5415	1786	2655	459	498	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P14902
A	-1	SER	-	expression tag	UNP P14902
A	0	HIS	-	expression tag	UNP P14902
B	-2	GLY	-	expression tag	UNP P14902
B	-1	SER	-	expression tag	UNP P14902
B	0	HIS	-	expression tag	UNP P14902
C	-2	GLY	-	expression tag	UNP P14902
C	-1	SER	-	expression tag	UNP P14902
C	0	HIS	-	expression tag	UNP P14902
D	-2	GLY	-	expression tag	UNP P14902
D	-1	SER	-	expression tag	UNP P14902
D	0	HIS	-	expression tag	UNP P14902

- Molecule 2 is N-(4-methylphenyl)-N'-[(1P,2'P)-4-propoxy-5-propyl-2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-3-yl]urea (CCD ID: Y9X) (formula: C₂₇H₃₀N₆O₂) (labeled as "Ligand of Interest" by depositor).

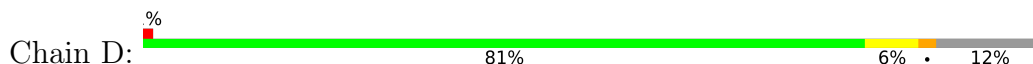


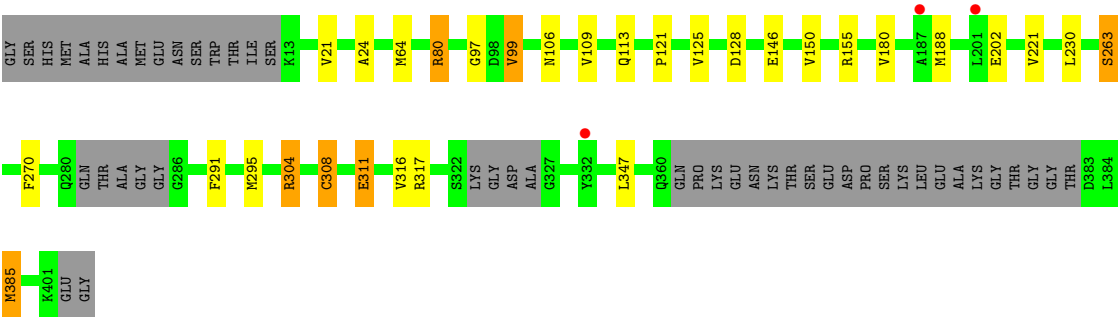
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	30	0
			65	27	30	6	2		
2	B	1	Total	C	H	N	O	30	0
			65	27	30	6	2		
2	C	1	Total	C	H	N	O	30	0
			65	27	30	6	2		
2	D	1	Total	C	H	N	O	30	0
			65	27	30	6	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	86	Total	O	0	0
			86	86		
3	C	75	Total	O	0	0
			75	75		
3	D	75	Total	O	0	0
			75	75		

- Molecule 1: Indoleamine 2,3-dioxygenase 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.88Å 120.29Å 100.82Å 90.00° 119.38° 90.00°	Depositor
Resolution (Å)	19.76 – 2.29 19.76 – 2.29	Depositor EDS
% Data completeness (in resolution range)	56.6 (19.76-2.29) 56.7 (19.76-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.28Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.279 , 0.300 (Not available) , 0.234	Depositor DCC
R_{free} test set	2839 reflections (2.96%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.428 for -h-2*k,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22495	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: Y9X

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	0.76	1/2869 (0.0%)	0.98	1/3897 (0.0%)
1	B	0.74	1/2886 (0.0%)	0.99	3/3920 (0.1%)
1	C	0.76	2/2806 (0.1%)	0.99	2/3810 (0.1%)
1	D	0.75	1/2825 (0.0%)	1.00	2/3842 (0.1%)
All	All	0.75	5/11386 (0.0%)	0.99	8/15469 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	64	MET	SD-CE	-8.22	1.59	1.79
1	D	64	MET	SD-CE	-7.94	1.59	1.79
1	A	64	MET	SD-CE	-7.90	1.59	1.79
1	C	148	MET	SD-CE	-6.34	1.63	1.79
1	B	148	MET	SD-CE	-5.94	1.64	1.79

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	VAL	CA-C-N	5.90	123.96	120.24
1	C	180	VAL	C-N-CA	5.90	123.96	120.24
1	B	180	VAL	CA-C-N	5.36	123.61	120.24
1	B	180	VAL	C-N-CA	5.36	123.61	120.24
1	D	125	VAL	CA-C-N	5.25	127.58	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2803	2723	2724	8	0
1	B	2819	2747	2747	10	0
1	C	2742	2669	2669	10	0
1	D	2760	2655	2655	13	0
2	A	35	30	0	1	0
2	B	35	30	0	1	0
2	C	35	30	0	0	0
2	D	35	30	0	0	0
3	A	81	0	0	0	0
3	B	86	0	0	0	0
3	C	75	0	0	0	0
3	D	75	0	0	1	0
All	All	11581	10914	10795	36	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.

The worst 5 of 36 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:C:80:ARG:NH1	1:C:121:PRO:O	2.14	0.81
1:D:21:VAL:HG12	1:D:24:ALA:HB3	1.67	0.77
1:B:21:VAL:HG12	1:B:24:ALA:HB3	1.68	0.73
1:D:21:VAL:CG1	1:D:24:ALA:HB3	2.24	0.68
1:B:21:VAL:CG1	1:B:24:ALA:HB3	2.25	0.67

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	356/406 (88%)	346 (97%)	10 (3%)	0	100	100
1	B	357/406 (88%)	345 (97%)	12 (3%)	0	100	100
1	C	343/406 (84%)	333 (97%)	9 (3%)	1 (0%)	36	44
1	D	350/406 (86%)	340 (97%)	10 (3%)	0	100	100
All	All	1406/1624 (87%)	1364 (97%)	41 (3%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	322	SER

5.3.2 Protein sidechains ⓘ

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	291/350 (83%)	277 (95%)	14 (5%)	23	32
1	B	294/350 (84%)	278 (95%)	16 (5%)	20	27
1	C	287/350 (82%)	271 (94%)	16 (6%)	19	25
1	D	284/350 (81%)	267 (94%)	17 (6%)	17	23
All	All	1156/1400 (83%)	1093 (95%)	63 (5%)	20	27

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	311	GLU
1	D	230	LEU
1	C	155	ARG
1	D	221	VAL
1	D	308	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	220	HIS
1	C	242	GLN
1	D	242	GLN
1	D	140	ASN
1	D	220	HIS

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](#)

4 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	Y9X	B	501	-	38,38,38	0.18	0	50,51,51	0.45	1 (2%)
2	Y9X	D	501	-	38,38,38	0.16	0	50,51,51	0.49	1 (2%)
2	Y9X	C	501	-	38,38,38	0.19	0	50,51,51	0.43	0
2	Y9X	A	501	-	38,38,38	0.20	0	50,51,51	0.60	1 (2%)

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	Y9X	B	501	-	-	3/23/23/23	0/4/4/4
2	Y9X	D	501	-	-	4/23/23/23	0/4/4/4
2	Y9X	C	501	-	-	4/23/23/23	0/4/4/4
2	Y9X	A	501	-	-	4/23/23/23	0/4/4/4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	Y9X	C27-O2-C18	3.28	124.08	114.22
2	B	501	Y9X	C27-O2-C18	2.09	120.48	114.22
2	D	501	Y9X	O2-C27-C26	-2.03	100.47	109.72

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	Y9X	C23-C26-C27-O2
2	A	501	Y9X	C26-C27-O2-C18
2	D	501	Y9X	C8-C16-N5-C20
2	D	501	Y9X	C7-C16-N5-C20
2	A	501	Y9X	C15-C18-O2-C27

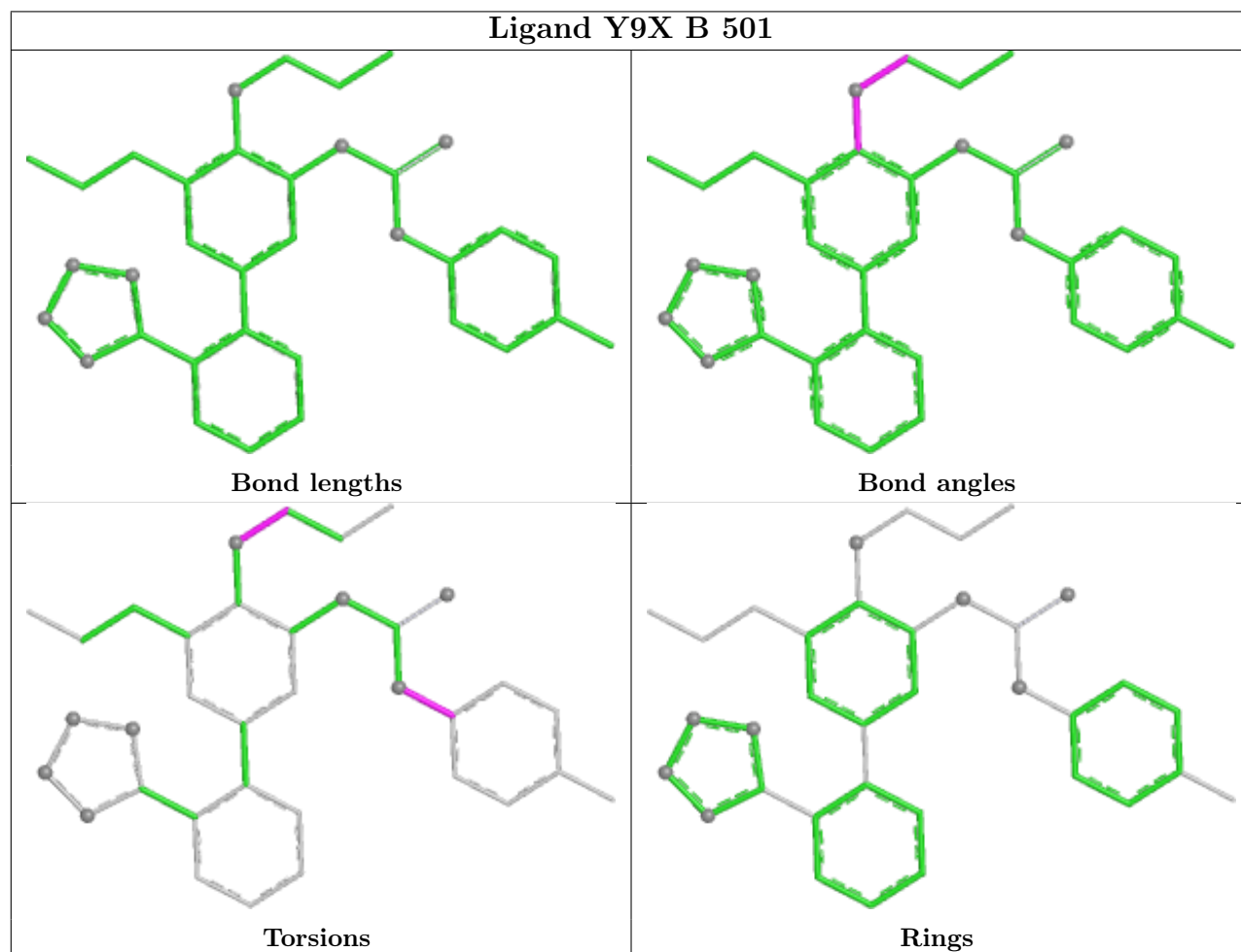
There are no ring outliers.

2 monomers are involved in 2 short contacts:

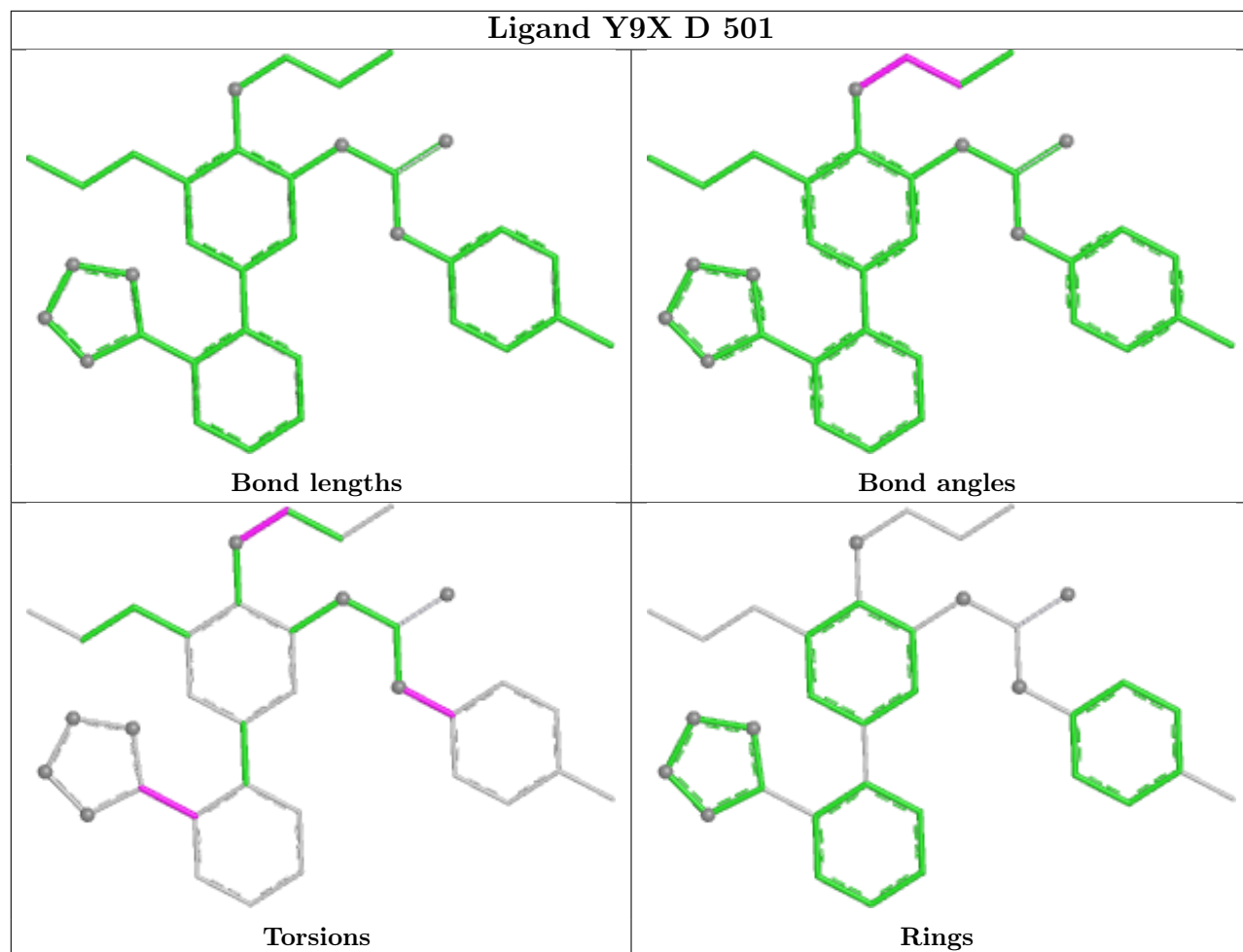
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	Y9X	1	0
2	A	501	Y9X	1	0

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

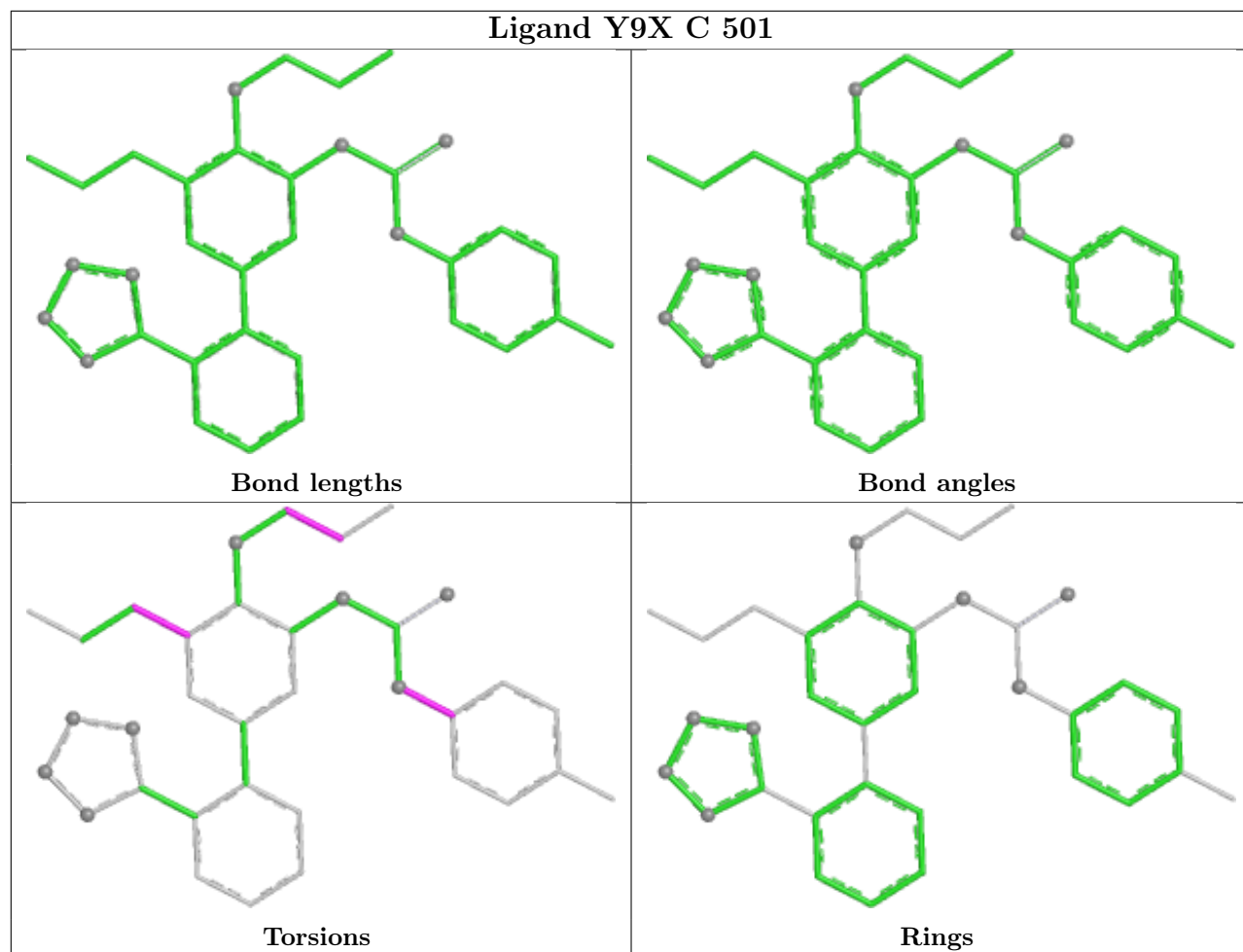
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

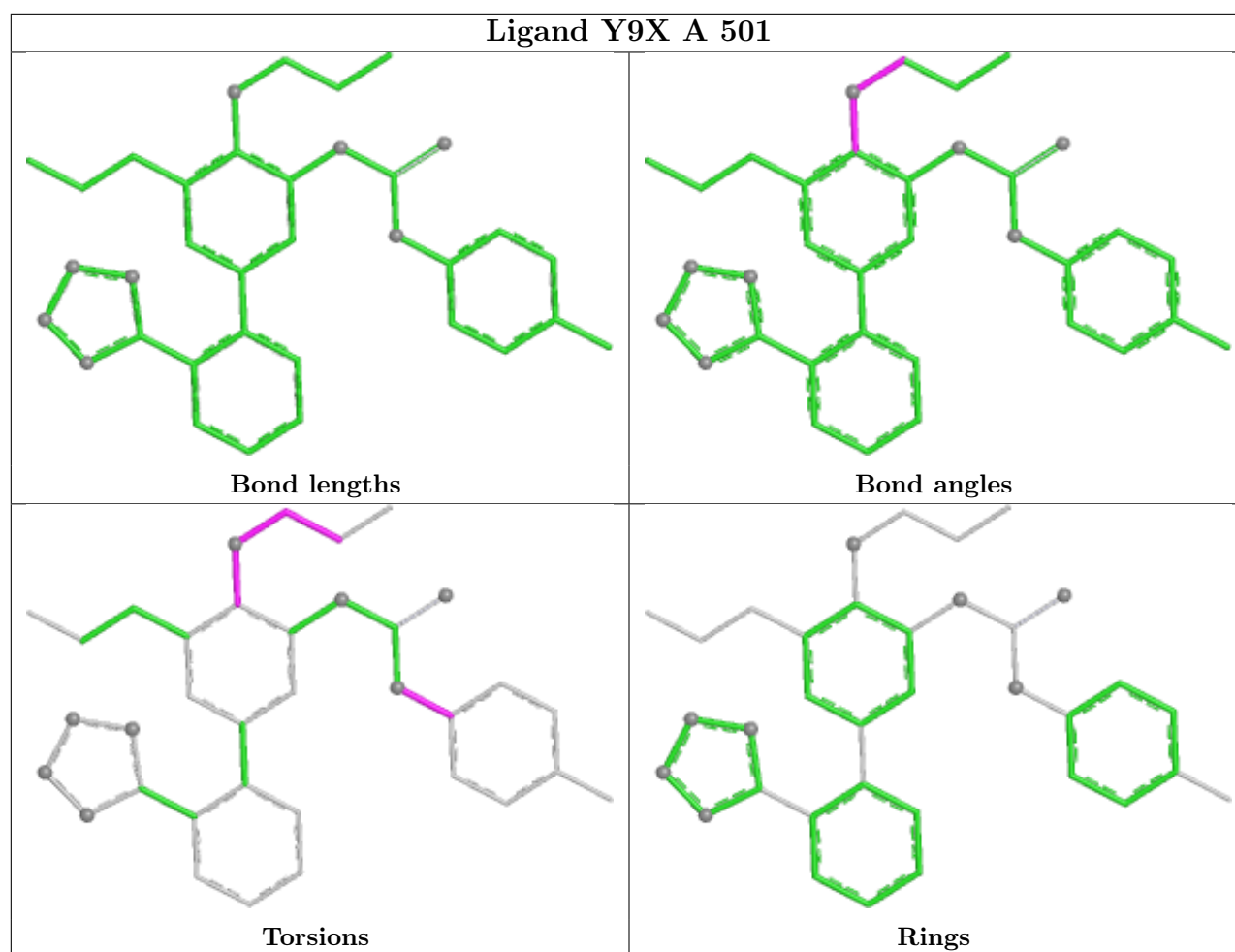


Ligand Y9X D 501



Ligand Y9X C 501





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	362/406 (89%)	-1.23	0	100 100	13, 27, 40, 56	0
1	B	363/406 (89%)	-1.23	0	100 100	13, 26, 40, 56	0
1	C	353/406 (86%)	-0.99	3 (0%)	82 84	13, 32, 66, 100	0
1	D	358/406 (88%)	-0.94	3 (0%)	82 84	15, 34, 70, 97	0
All	All	1436/1624 (88%)	-1.10	6 (0%)	88 89	13, 29, 60, 100	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	316	VAL	3.4
1	C	184	VAL	3.3
1	D	201	LEU	2.4
1	D	332	TYR	2.2
1	C	328	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

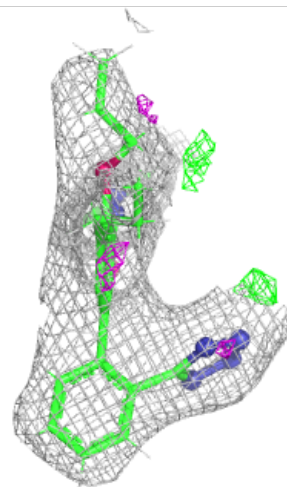
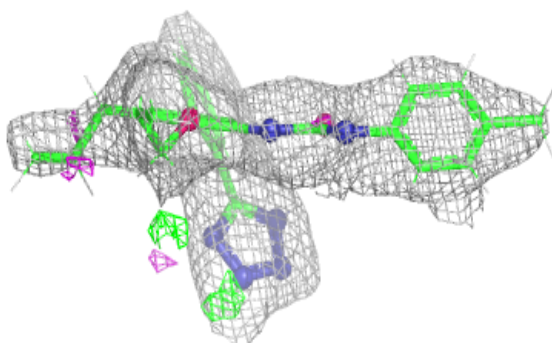
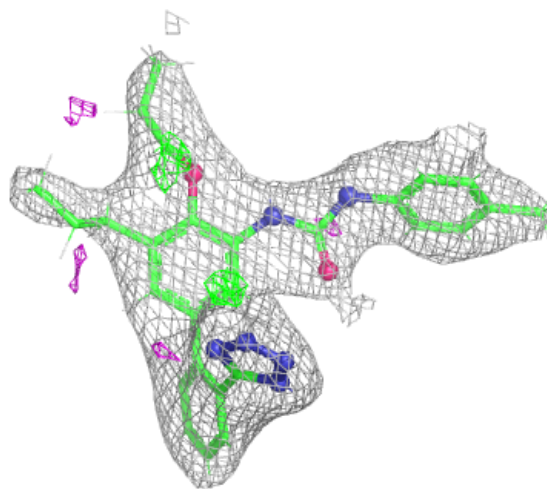
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	Y9X	A	501	35/35	0.98	0.04	45,47,48,48	30
2	Y9X	B	501	35/35	0.98	0.04	43,44,44,44	30
2	Y9X	C	501	35/35	0.98	0.04	60,62,62,62	30
2	Y9X	D	501	35/35	0.99	0.04	64,65,67,67	30

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.

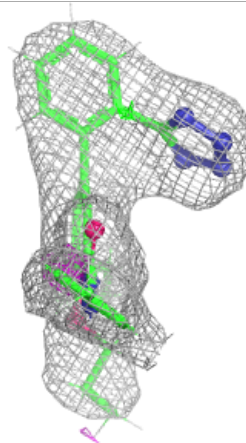
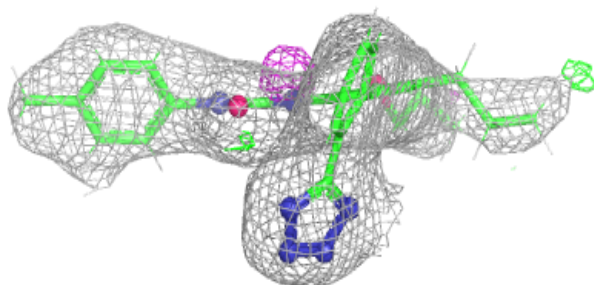
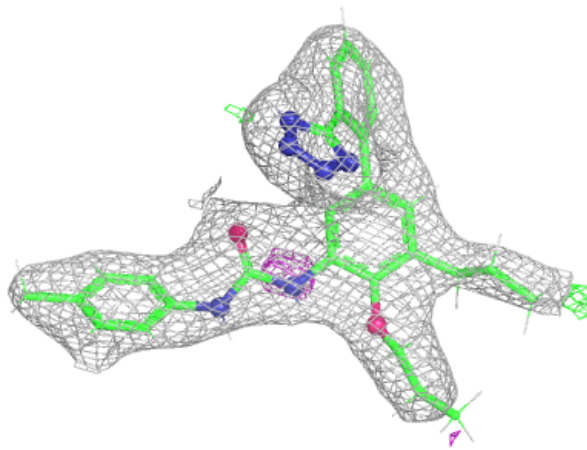
Electron density around Y9X A 501:

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



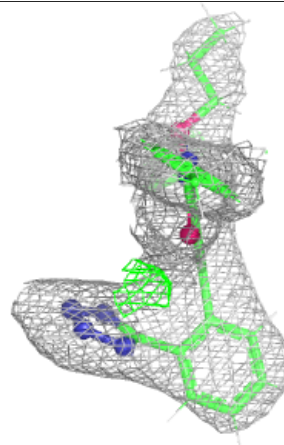
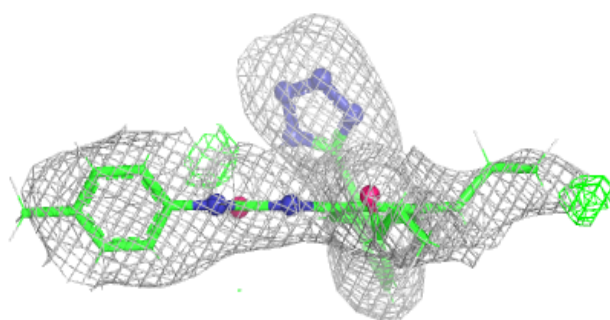
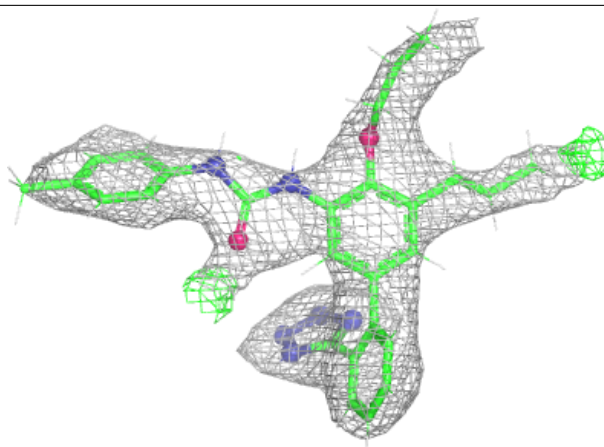
Electron density around Y9X B 501:

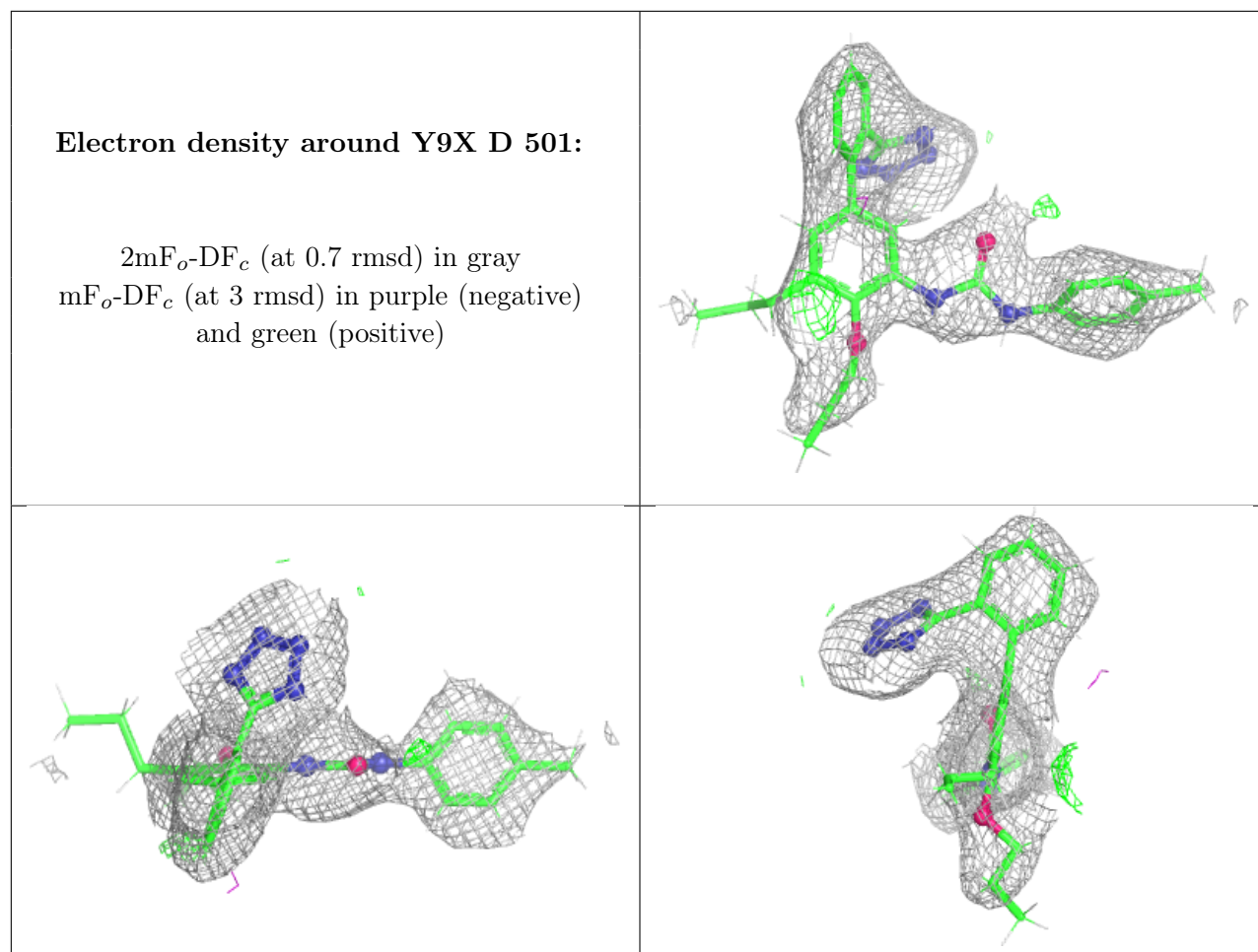
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Y9X C 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.