



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:16 AM UTC

PDB ID : 8R5R / pdb_00008r5r
Title : Structure of apo TDO with a bound inhibitor
Authors : Wicki, M.; Mac Sweeney, A.
Deposited on : 2023-11-17
Resolution : 3.08 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 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

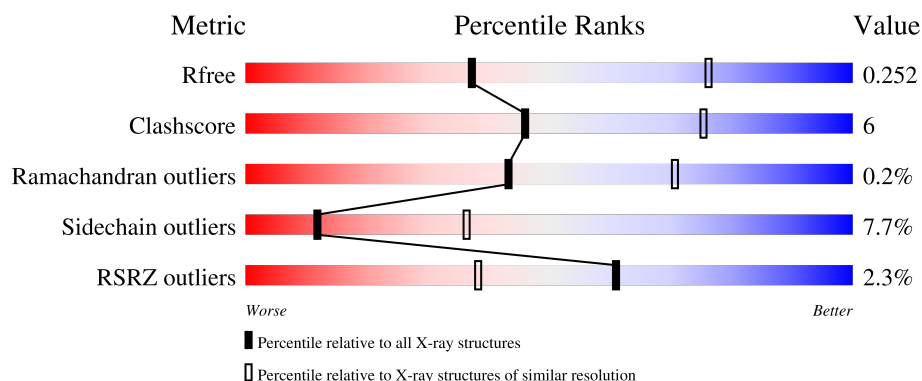
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	358	 3% 70% 16% • 12%
1	B	358	 3% 73% 15% • 11%
1	C	358	 % 73% 14% • 11%
1	D	358	 % 75% 11% • 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10002 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
1	A	314	Total	C	N	O	S	0	0	0
			2512	1628	428	446	10			
1	B	318	Total	C	N	O	S	0	0	0
			2522	1634	430	448	10			
1	C	317	Total	C	N	O	S	0	0	0
			2471	1596	426	439	10			
1	D	314	Total	C	N	O	S	0	0	0
			2334	1504	402	418	10			

There are 28 discrepancies between the modelled and reference sequences:

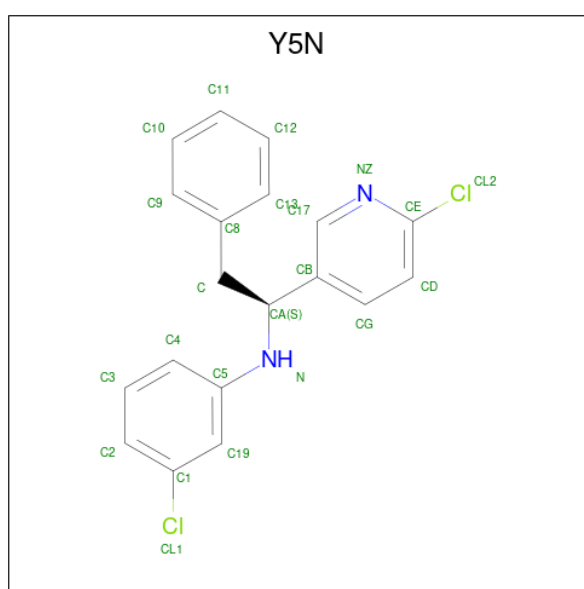
Chain	Residue	Modelled	Actual	Comment	Reference
A	390	GLU	-	expression tag	UNP P48775
A	391	HIS	-	expression tag	UNP P48775
A	392	HIS	-	expression tag	UNP P48775
A	393	HIS	-	expression tag	UNP P48775
A	394	HIS	-	expression tag	UNP P48775
A	395	HIS	-	expression tag	UNP P48775
A	396	HIS	-	expression tag	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
B	394	HIS	-	expression tag	UNP P48775
B	395	HIS	-	expression tag	UNP P48775
B	396	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
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775

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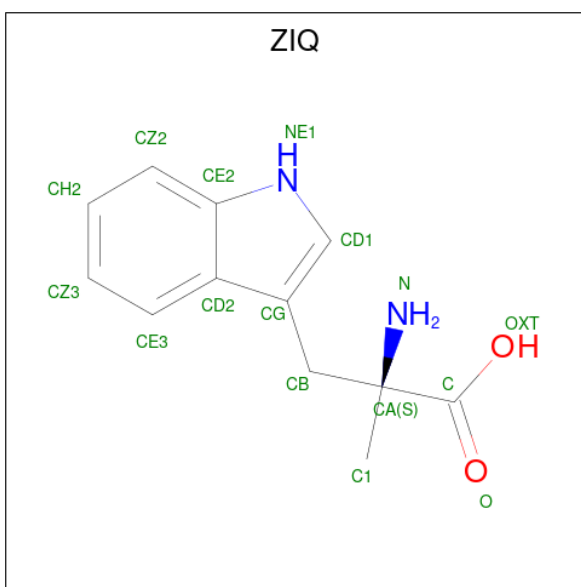
Chain	Residue	Modelled	Actual	Comment	Reference
D	390	GLU	-	expression tag	UNP P48775
D	391	HIS	-	expression tag	UNP P48775
D	392	HIS	-	expression tag	UNP P48775
D	393	HIS	-	expression tag	UNP P48775
D	394	HIS	-	expression tag	UNP P48775
D	395	HIS	-	expression tag	UNP P48775
D	396	HIS	-	expression tag	UNP P48775

- Molecule 2 is 3-chloranyl- {N}-[(1 {S})-1-(6-chloranypyridin-3-yl)-2-phenyl-ethyl]aniline (CCD ID: Y5N) (formula: C₁₉H₁₆Cl₂N₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			23	19	2	2		
2	B	1	Total	C	Cl	N	0	0
			23	19	2	2		
2	C	1	Total	C	Cl	N	0	0
			23	19	2	2		
2	D	1	Total	C	Cl	N	0	0
			23	19	2	2		

- Molecule 3 is alpha-methyl-L-tryptophan (CCD ID: ZIQ) (formula: C₁₂H₁₄N₂O₂).



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

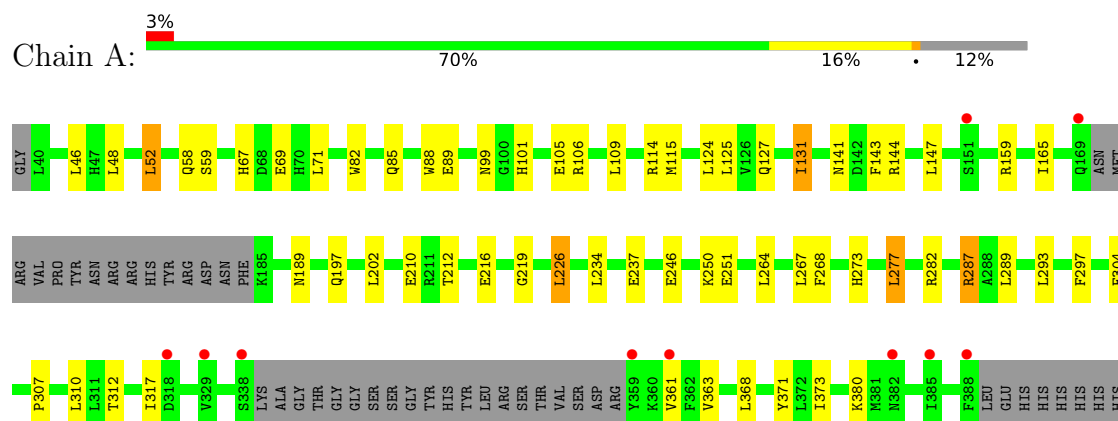
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	4	Total	O	0	0
			4	4		

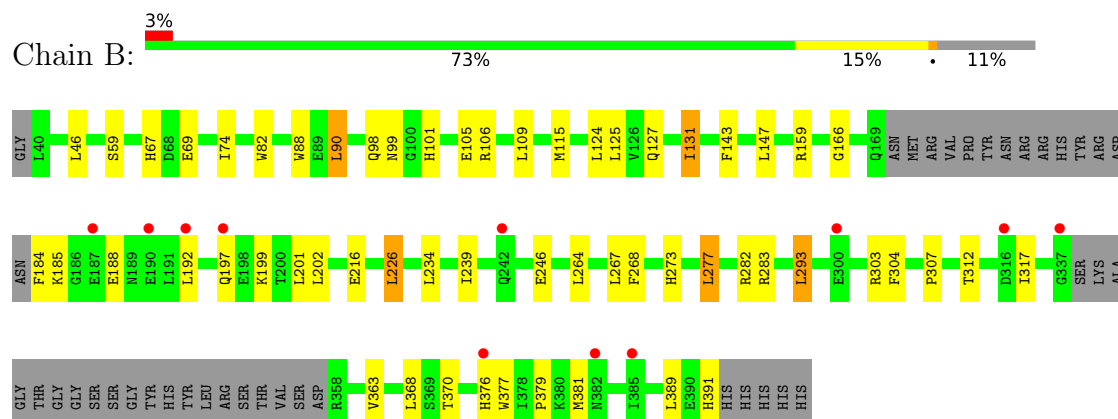
3 Residue-property plots

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.

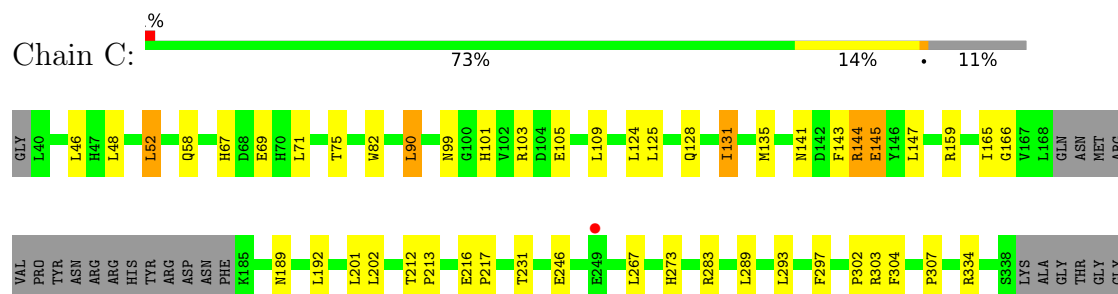
• Molecule 1: Tryptophan 2,3-dioxygenase

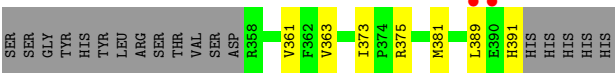


• Molecule 1: Tryptophan 2,3-dioxygenase

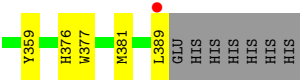
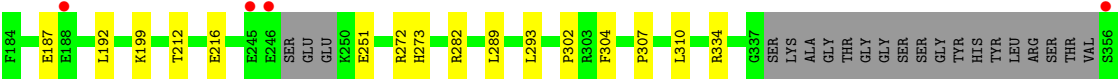
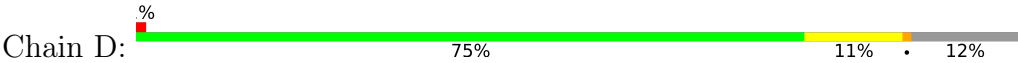


• Molecule 1: Tryptophan 2,3-dioxygenase





● Molecule 1: Tryptophan 2,3-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.74Å 132.91Å 137.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.83 – 3.08 50.83 – 3.08	Depositor EDS
% Data completeness (in resolution range)	87.0 (50.83-3.08) 87.0 (50.83-3.08)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.227 , 0.252 0.230 , 0.252	Depositor DCC
R_{free} test set	1368 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	85.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10002	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: Y5N, ZIQ

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	0.65	0/2568	1.10	3/3475 (0.1%)
1	B	0.67	0/2580	1.11	3/3491 (0.1%)
1	C	0.66	0/2528	1.09	1/3431 (0.0%)
1	D	0.66	0/2388	1.09	2/3248 (0.1%)
All	All	0.66	0/10064	1.10	9/13645 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	141	ASN	CA-CB-CG	5.86	118.46	112.60
1	B	184	PHE	CA-CB-CG	5.64	119.44	113.80
1	B	312	THR	CA-C-N	5.57	127.75	120.28
1	B	312	THR	C-N-CA	5.57	127.75	120.28
1	C	144	ARG	N-CA-C	-5.57	102.03	110.28
1	A	312	THR	CA-C-N	5.56	127.73	120.28
1	A	312	THR	C-N-CA	5.56	127.73	120.28
1	D	359	TYR	N-CA-C	-5.45	104.08	111.55
1	A	371	TYR	N-CA-C	-5.19	100.62	108.67

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	2512	0	2404	35	0
1	B	2522	0	2381	33	0
1	C	2471	0	2284	32	0
1	D	2334	0	2001	25	0
2	A	23	0	0	1	0
2	B	23	0	0	1	0
2	C	23	0	0	1	0
2	D	23	0	0	1	0
3	A	16	0	0	1	0
3	B	16	0	0	0	0
3	C	16	0	0	1	0
3	D	16	0	0	1	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0
All	All	10002	0	9070	110	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 6.

All (110) 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:141:ASN:HA	1:C:144:ARG:HG2	1.48	0.95
1:D:273:HIS:CE1	1:D:289:LEU:HD11	2.06	0.90
1:A:273:HIS:CE1	1:A:289:LEU:HD11	2.10	0.86
1:C:273:HIS:CE1	1:C:289:LEU:HD11	2.12	0.85
1:D:141:ASN:HA	1:D:144:ARG:CG	2.11	0.81
1:B:159:ARG:HG2	1:B:192:LEU:HD21	1.65	0.78
1:C:141:ASN:HA	1:C:144:ARG:CG	2.12	0.78
1:A:99:ASN:HD21	1:A:101:HIS:CD2	2.05	0.75
1:B:99:ASN:HD21	1:B:101:HIS:CD2	2.06	0.73
1:C:99:ASN:HD21	1:C:101:HIS:CD2	2.08	0.70
1:D:273:HIS:NE2	1:D:289:LEU:HD11	2.05	0.70
1:C:273:HIS:NE2	1:C:289:LEU:HD11	2.12	0.65
1:D:141:ASN:HA	1:D:144:ARG:HG3	1.78	0.65
1:A:273:HIS:NE2	1:A:289:LEU:HD11	2.12	0.64
1:D:141:ASN:HA	1:D:144:ARG:HG2	1.78	0.63
1:B:185:LYS:HB3	1:B:188:GLU:HB2	1.82	0.60
1:C:135:MET:O	1:C:334:ARG:NH2	2.34	0.60
1:D:98:GLN:HE21	1:D:199:LYS:HE3	1.67	0.59
1:A:277:LEU:HD12	1:A:282:ARG:HB3	1.85	0.58
1:D:135:MET:O	1:D:334:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LEU:HG	1:B:368:LEU:HD22	1.86	0.57
1:C:144:ARG:O	1:C:145:GLU:CB	2.52	0.57
1:A:106:ARG:HG2	1:C:302:PRO:HD3	1.86	0.57
1:C:141:ASN:CA	1:C:144:ARG:HG2	2.30	0.57
1:C:46:LEU:HD21	2:D:501:Y5N:CL1	2.41	0.56
1:B:277:LEU:HD12	1:B:282:ARG:HB3	1.87	0.56
1:C:48:LEU:HB3	1:C:52:LEU:HD22	1.88	0.55
1:A:210:GLU:HG2	1:A:287:ARG:HB3	1.90	0.54
1:B:166:GLY:O	1:B:283:ARG:NH2	2.39	0.53
1:C:131:ILE:HD13	1:D:124:LEU:HD22	1.91	0.53
1:C:124:LEU:HD22	1:D:131:ILE:HD13	1.90	0.53
1:B:90:LEU:HD21	1:B:201:LEU:HD22	1.91	0.53
1:A:131:ILE:HD13	1:B:124:LEU:HD22	1.90	0.53
1:C:166:GLY:O	1:C:283:ARG:NH2	2.40	0.52
1:A:99:ASN:ND2	1:A:101:HIS:CD2	2.76	0.52
1:B:98:GLN:HE21	1:B:199:LYS:HE3	1.74	0.52
2:C:501:Y5N:CL1	1:D:46:LEU:HD21	2.47	0.51
1:A:48:LEU:HB3	1:A:52:LEU:HD22	1.92	0.51
1:D:381:MET:HE1	1:D:389:LEU:HD12	1.92	0.51
1:C:202:LEU:HD21	1:C:283:ARG:HB3	1.93	0.51
1:B:226:LEU:HD13	1:B:268:PHE:HZ	1.75	0.51
1:C:90:LEU:HD21	1:C:201:LEU:HD22	1.93	0.51
1:B:99:ASN:ND2	1:B:101:HIS:CD2	2.76	0.50
1:A:226:LEU:HD13	1:A:268:PHE:HZ	1.76	0.49
1:B:381:MET:HE1	1:B:389:LEU:HD12	1.93	0.49
1:A:124:LEU:HD22	1:B:131:ILE:HD13	1.94	0.49
1:B:106:ARG:HG2	1:D:302:PRO:HD3	1.93	0.49
1:A:212:THR:HG22	3:A:502:ZIQ:CZ2	2.43	0.49
1:D:80:GLU:HG3	1:D:157:GLN:HE21	1.77	0.49
1:B:303:ARG:HA	1:B:391:HIS:CE1	2.48	0.48
1:A:46:LEU:HD21	2:B:501:Y5N:CL1	2.51	0.48
1:D:212:THR:HG22	3:D:502:ZIQ:CZ2	2.44	0.48
1:A:293:LEU:HD13	1:A:368:LEU:HD22	1.96	0.48
1:B:303:ARG:HA	1:B:391:HIS:HE1	1.79	0.47
1:C:304:PHE:C	1:C:307:PRO:HD2	2.40	0.47
1:A:88:TRP:CD1	1:B:67:HIS:CE1	3.03	0.47
1:A:124:LEU:HD22	1:B:131:ILE:CD1	2.45	0.47
1:C:297:PHE:HZ	1:C:373:ILE:HD12	1.80	0.47
1:A:69:GLU:HG3	1:A:143:PHE:CD1	2.50	0.46
2:A:501:Y5N:CL1	1:B:46:LEU:HD21	2.52	0.46
1:D:216:GLU:CD	1:D:216:GLU:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLN:NE2	1:A:89:GLU:OE2	2.49	0.46
1:C:67:HIS:CD2	1:D:114:ARG:CZ	2.97	0.46
1:C:75:THR:HG23	1:C:128:GLN:HE21	1.81	0.46
1:C:99:ASN:ND2	1:C:101:HIS:CD2	2.79	0.46
1:A:304:PHE:C	1:A:307:PRO:HD2	2.41	0.46
1:C:202:LEU:HD21	1:C:283:ARG:CB	2.46	0.46
1:B:82:TRP:CB	1:B:125:LEU:HD21	2.46	0.45
1:C:381:MET:HE1	1:C:389:LEU:HD12	1.98	0.45
1:D:69:GLU:HG3	1:D:143:PHE:CD1	2.51	0.45
1:D:376:HIS:ND1	1:D:377:TRP:CD1	2.84	0.45
1:C:165:ILE:HG22	1:C:361:VAL:HG21	1.98	0.45
1:C:69:GLU:HG3	1:C:143:PHE:CD1	2.52	0.45
1:B:273:HIS:CE1	1:B:277:LEU:CD1	3.00	0.44
1:A:293:LEU:HD13	1:A:368:LEU:HB3	1.99	0.44
1:D:304:PHE:C	1:D:307:PRO:HD2	2.42	0.44
1:A:82:TRP:CB	1:A:125:LEU:HD21	2.48	0.44
1:B:69:GLU:HG3	1:B:143:PHE:CD1	2.52	0.44
1:B:304:PHE:C	1:B:307:PRO:HD2	2.42	0.44
1:A:273:HIS:CE1	1:A:277:LEU:CD1	3.00	0.44
1:A:297:PHE:HZ	1:A:373:ILE:HD12	1.83	0.44
1:C:99:ASN:ND2	1:C:101:HIS:NE2	2.66	0.44
1:A:114:ARG:CZ	1:B:67:HIS:CD2	3.00	0.44
1:D:57:LEU:HD21	1:D:70:HIS:HA	1.99	0.44
1:C:303:ARG:HA	1:C:391:HIS:CE1	2.53	0.43
1:A:82:TRP:CH2	1:B:131:ILE:HG21	2.52	0.43
1:B:234:LEU:HD21	1:B:264:LEU:HD12	2.00	0.43
1:B:273:HIS:NE2	1:B:277:LEU:CD1	2.81	0.43
1:A:234:LEU:HD21	1:A:264:LEU:HD12	2.00	0.42
1:C:103:ARG:HA	3:C:502:ZIQ:OXT	2.19	0.42
1:C:212:THR:HA	1:C:213:PRO:HD3	1.94	0.42
1:A:165:ILE:HG22	1:A:361:VAL:HG21	2.01	0.42
1:A:115:MET:HE3	1:A:317:ILE:CD1	2.49	0.42
1:A:99:ASN:ND2	1:A:101:HIS:NE2	2.68	0.42
1:C:216:GLU:HA	1:C:217:PRO:HD3	1.95	0.42
1:A:71:LEU:HD11	1:A:131:ILE:HG23	2.01	0.42
1:A:67:HIS:CE1	1:B:88:TRP:CD1	3.07	0.42
1:A:273:HIS:NE2	1:A:277:LEU:CD1	2.82	0.42
1:A:141:ASN:OD1	1:A:144:ARG:NH1	2.53	0.42
1:C:82:TRP:CB	1:C:125:LEU:HD21	2.50	0.41
1:C:67:HIS:CE1	1:D:88:TRP:CD1	3.08	0.41
1:D:85:GLN:NE2	1:D:89:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:TRP:CB	1:D:125:LEU:HD21	2.49	0.41
1:B:115:MET:HE3	1:B:317:ILE:CD1	2.51	0.41
1:D:141:ASN:CA	1:D:144:ARG:HG3	2.46	0.41
1:B:376:HIS:ND1	1:B:377:TRP:CD1	2.88	0.41
1:A:88:TRP:NE1	1:B:67:HIS:CE1	2.89	0.41
1:B:226:LEU:HD23	1:B:379:PRO:HD3	2.02	0.41
1:D:376:HIS:ND1	1:D:377:TRP:HD1	2.18	0.41
1:A:85:GLN:HB2	1:B:74:ILE:HG21	2.02	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	308/358 (86%)	299 (97%)	8 (3%)	1 (0%)	36	64
1	B	312/358 (87%)	301 (96%)	11 (4%)	0	100	100
1	C	311/358 (87%)	300 (96%)	10 (3%)	1 (0%)	36	64
1	D	306/358 (86%)	295 (96%)	11 (4%)	0	100	100
All	All	1237/1432 (86%)	1195 (97%)	40 (3%)	2 (0%)	43	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	145	GLU
1	A	219	GLY

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	255/330 (77%)	231 (91%)	24 (9%)	8	29
1	B	252/330 (76%)	234 (93%)	18 (7%)	13	39
1	C	240/330 (73%)	223 (93%)	17 (7%)	13	39
1	D	198/330 (60%)	184 (93%)	14 (7%)	13	39
All	All	945/1320 (72%)	872 (92%)	73 (8%)	12	36

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	58	GLN
1	A	59	SER
1	A	105	GLU
1	A	109	LEU
1	A	127	GLN
1	A	131	ILE
1	A	147	LEU
1	A	159	ARG
1	A	189	ASN
1	A	197	GLN
1	A	202	LEU
1	A	216	GLU
1	A	226	LEU
1	A	237	GLU
1	A	246	GLU
1	A	250	LYS
1	A	251	GLU
1	A	267	LEU
1	A	277	LEU
1	A	287	ARG
1	A	310	LEU
1	A	363	VAL
1	A	380	LYS
1	B	59	SER
1	B	90	LEU
1	B	105	GLU
1	B	109	LEU

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Mol	Chain	Res	Type
1	B	127	GLN
1	B	131	ILE
1	B	147	LEU
1	B	197	GLN
1	B	202	LEU
1	B	216	GLU
1	B	226	LEU
1	B	239	ILE
1	B	246	GLU
1	B	267	LEU
1	B	277	LEU
1	B	293	LEU
1	B	363	VAL
1	B	370	THR
1	C	52	LEU
1	C	58	GLN
1	C	71	LEU
1	C	90	LEU
1	C	105	GLU
1	C	109	LEU
1	C	131	ILE
1	C	147	LEU
1	C	159	ARG
1	C	189	ASN
1	C	192	LEU
1	C	231	THR
1	C	246	GLU
1	C	267	LEU
1	C	293	LEU
1	C	363	VAL
1	C	375	ARG
1	D	58	GLN
1	D	65	LYS
1	D	80	GLU
1	D	105	GLU
1	D	131	ILE
1	D	144	ARG
1	D	147	LEU
1	D	187	GLU
1	D	192	LEU
1	D	251	GLU
1	D	272	ARG

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Mol	Chain	Res	Type
1	D	282	ARG
1	D	293	LEU
1	D	310	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	101	HIS
1	A	154	GLN
1	A	258	GLN
1	A	275	HIS
1	A	309	GLN
1	A	327	ASN
1	A	328	HIS
1	B	98	GLN
1	B	99	ASN
1	B	101	HIS
1	B	127	GLN
1	B	154	GLN
1	B	309	GLN
1	B	391	HIS
1	C	58	GLN
1	C	99	ASN
1	C	101	HIS
1	C	128	GLN
1	C	154	GLN
1	C	275	HIS
1	C	309	GLN
1	C	327	ASN
1	C	328	HIS
1	C	382	ASN
1	C	391	HIS
1	D	55	GLN
1	D	98	GLN
1	D	141	ASN
1	D	154	GLN
1	D	275	HIS
1	D	309	GLN
1	D	382	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	ZIQ	A	502	-	14,17,17	1.47	3 (21%)	20,25,25	1.62	4 (20%)
2	Y5N	D	501	-	25,25,25	0.27	0	31,33,33	0.31	0
3	ZIQ	D	502	-	14,17,17	1.44	2 (14%)	20,25,25	1.51	4 (20%)
2	Y5N	C	501	-	25,25,25	0.25	0	31,33,33	0.29	0
3	ZIQ	B	502	-	14,17,17	1.51	2 (14%)	20,25,25	1.43	3 (15%)
2	Y5N	B	501	-	25,25,25	0.41	0	31,33,33	0.34	0
2	Y5N	A	501	-	25,25,25	0.25	0	31,33,33	0.33	0
3	ZIQ	C	502	-	14,17,17	1.52	4 (28%)	20,25,25	1.42	3 (15%)

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	ZIQ	A	502	-	-	4/11/11/11	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y5N	D	501	-	-	0/12/12/12	0/3/3/3
3	ZIQ	D	502	-	-	3/11/11/11	0/2/2/2
2	Y5N	C	501	-	-	0/12/12/12	0/3/3/3
3	ZIQ	B	502	-	-	5/11/11/11	0/2/2/2
2	Y5N	B	501	-	-	0/12/12/12	0/3/3/3
2	Y5N	A	501	-	-	0/12/12/12	0/3/3/3
3	ZIQ	C	502	-	-	3/11/11/11	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	ZIQ	CD2-CG	-3.28	1.38	1.44
3	B	502	ZIQ	CD2-CG	-3.16	1.38	1.44
3	C	502	ZIQ	CD2-CG	-3.14	1.38	1.44
3	A	502	ZIQ	CD2-CG	-3.08	1.38	1.44
3	B	502	ZIQ	CD2-CE2	-2.62	1.38	1.41
3	C	502	ZIQ	CD2-CE2	-2.29	1.38	1.41
3	A	502	ZIQ	CD2-CE2	-2.24	1.38	1.41
3	A	502	ZIQ	CD1-CG	2.22	1.40	1.36
3	C	502	ZIQ	CB-CA	-2.16	1.52	1.55
3	C	502	ZIQ	CE2-NE1	-2.10	1.34	1.37
3	D	502	ZIQ	CD2-CE2	-2.03	1.38	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	ZIQ	CZ2-CE2-CD2	-3.98	118.34	122.19
3	B	502	ZIQ	CZ2-CE2-CD2	-3.35	118.95	122.19
3	D	502	ZIQ	CZ2-CE2-CD2	-3.25	119.04	122.19
3	D	502	ZIQ	CE3-CD2-CE2	3.10	122.05	118.84
3	C	502	ZIQ	CZ2-CE2-CD2	-3.03	119.25	122.19
3	B	502	ZIQ	CE3-CD2-CE2	3.02	121.97	118.84
3	C	502	ZIQ	CE3-CD2-CE2	2.95	121.90	118.84
3	D	502	ZIQ	CE3-CD2-CG	-2.95	129.45	133.85
3	A	502	ZIQ	CE3-CD2-CE2	2.94	121.88	118.84
3	A	502	ZIQ	CE3-CD2-CG	-2.85	129.60	133.85
3	D	502	ZIQ	O-C-CA	-2.74	117.86	122.78
3	B	502	ZIQ	CE3-CD2-CG	-2.72	129.79	133.85
3	C	502	ZIQ	CE3-CD2-CG	-2.68	129.86	133.85
3	A	502	ZIQ	O-C-CA	-2.59	118.13	122.78

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	ZIQ	CA-CB-CG-CD2
3	A	502	ZIQ	OXT-C-CA-C1
3	B	502	ZIQ	OXT-C-CA-C1
3	A	502	ZIQ	O-C-CA-CB
3	A	502	ZIQ	OXT-C-CA-CB
3	B	502	ZIQ	O-C-CA-CB
3	B	502	ZIQ	OXT-C-CA-CB
3	C	502	ZIQ	O-C-CA-CB
3	C	502	ZIQ	OXT-C-CA-CB
3	D	502	ZIQ	OXT-C-CA-CB
3	C	502	ZIQ	O-C-CA-N
3	D	502	ZIQ	O-C-CA-N
3	A	502	ZIQ	CA-CB-CG-CD2
3	B	502	ZIQ	CA-CB-CG-CD1
3	D	502	ZIQ	O-C-CA-CB

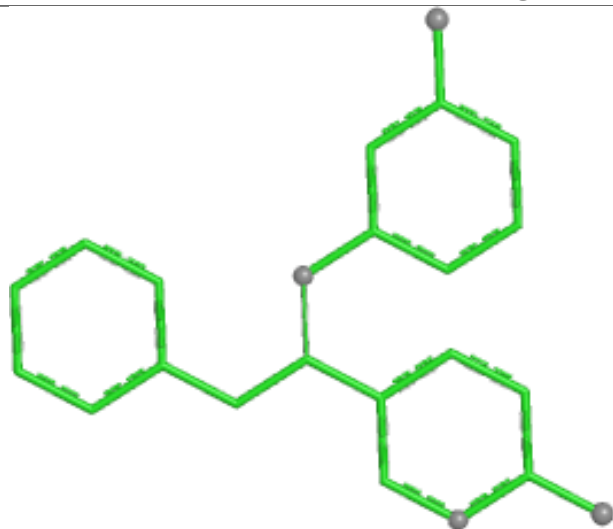
There are no ring outliers.

7 monomers are involved in 7 short contacts:

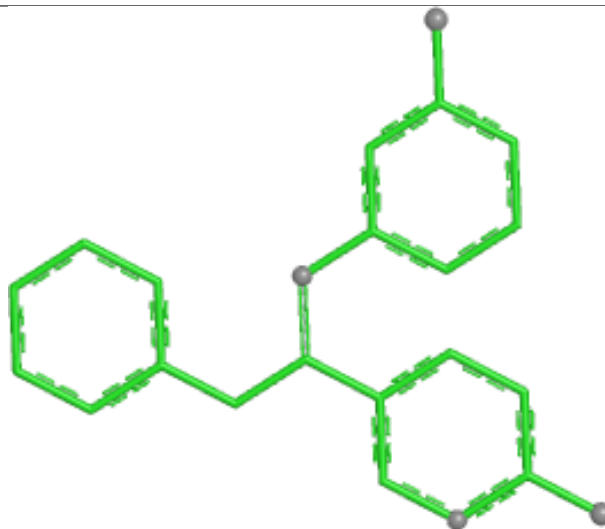
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	ZIQ	1	0
2	D	501	Y5N	1	0
3	D	502	ZIQ	1	0
2	C	501	Y5N	1	0
2	B	501	Y5N	1	0
2	A	501	Y5N	1	0
3	C	502	ZIQ	1	0

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.

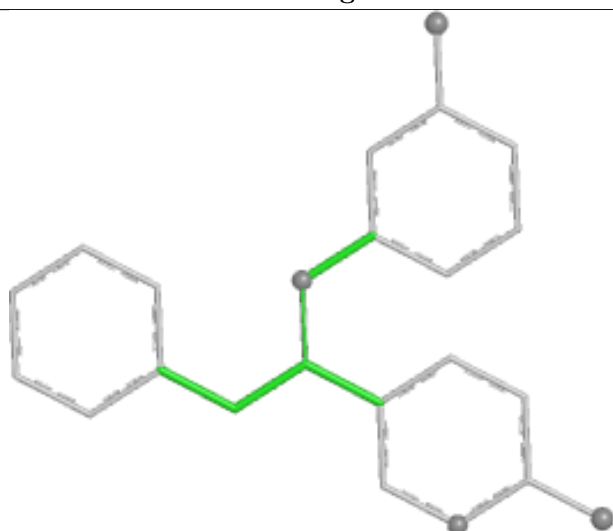
Ligand Y5N D 501



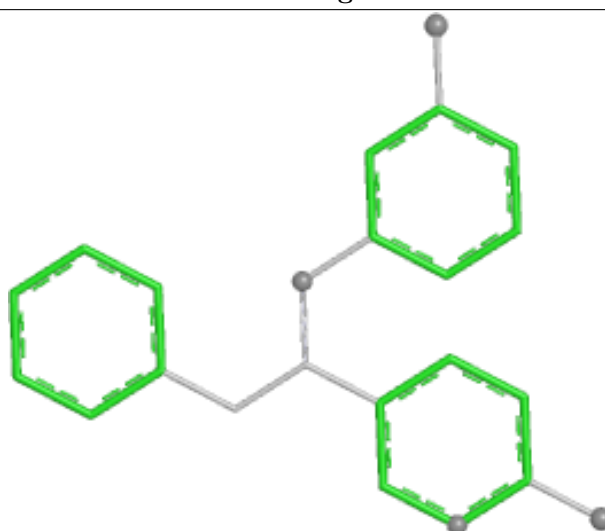
Bond lengths



Bond angles

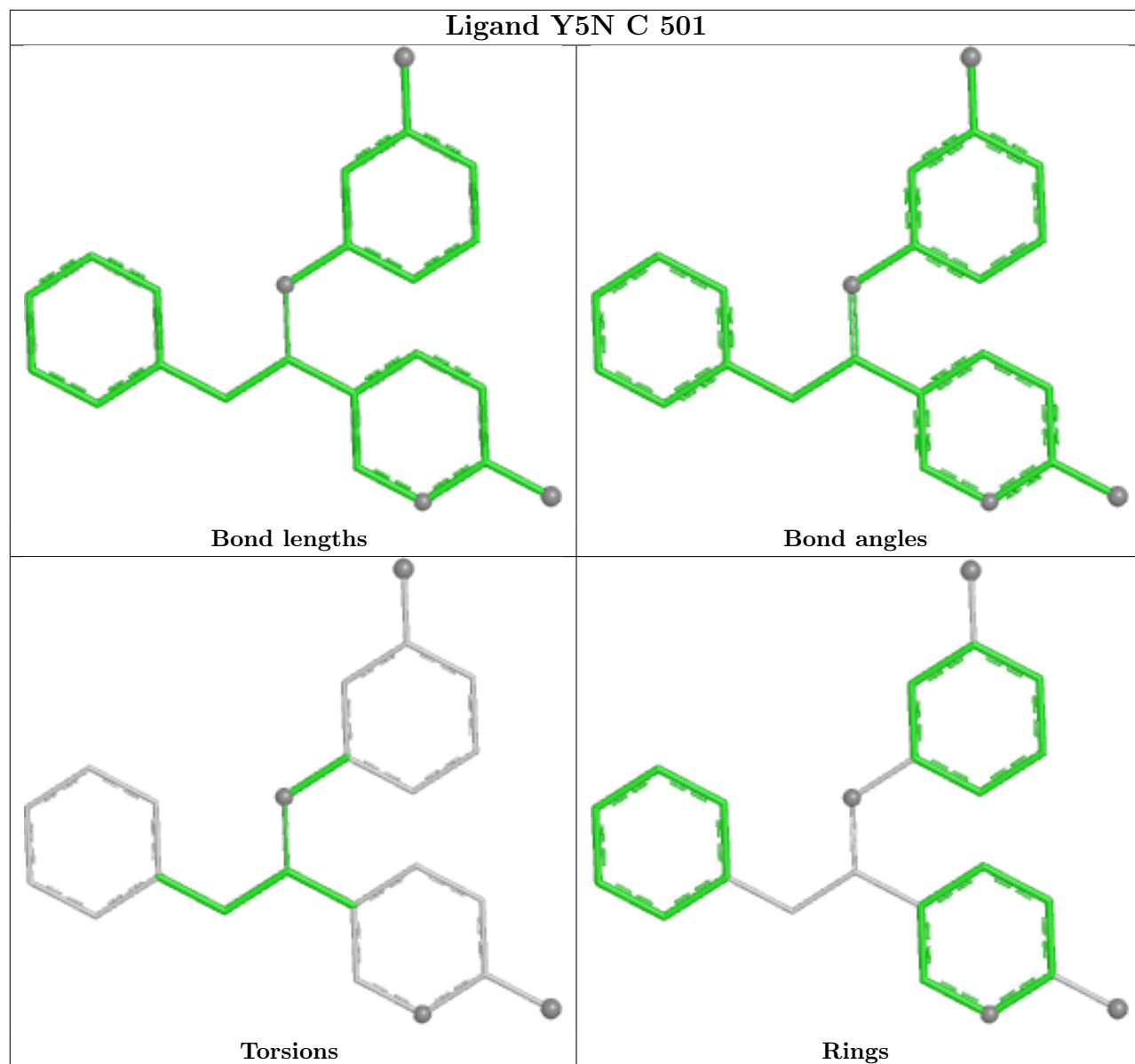


Torsions

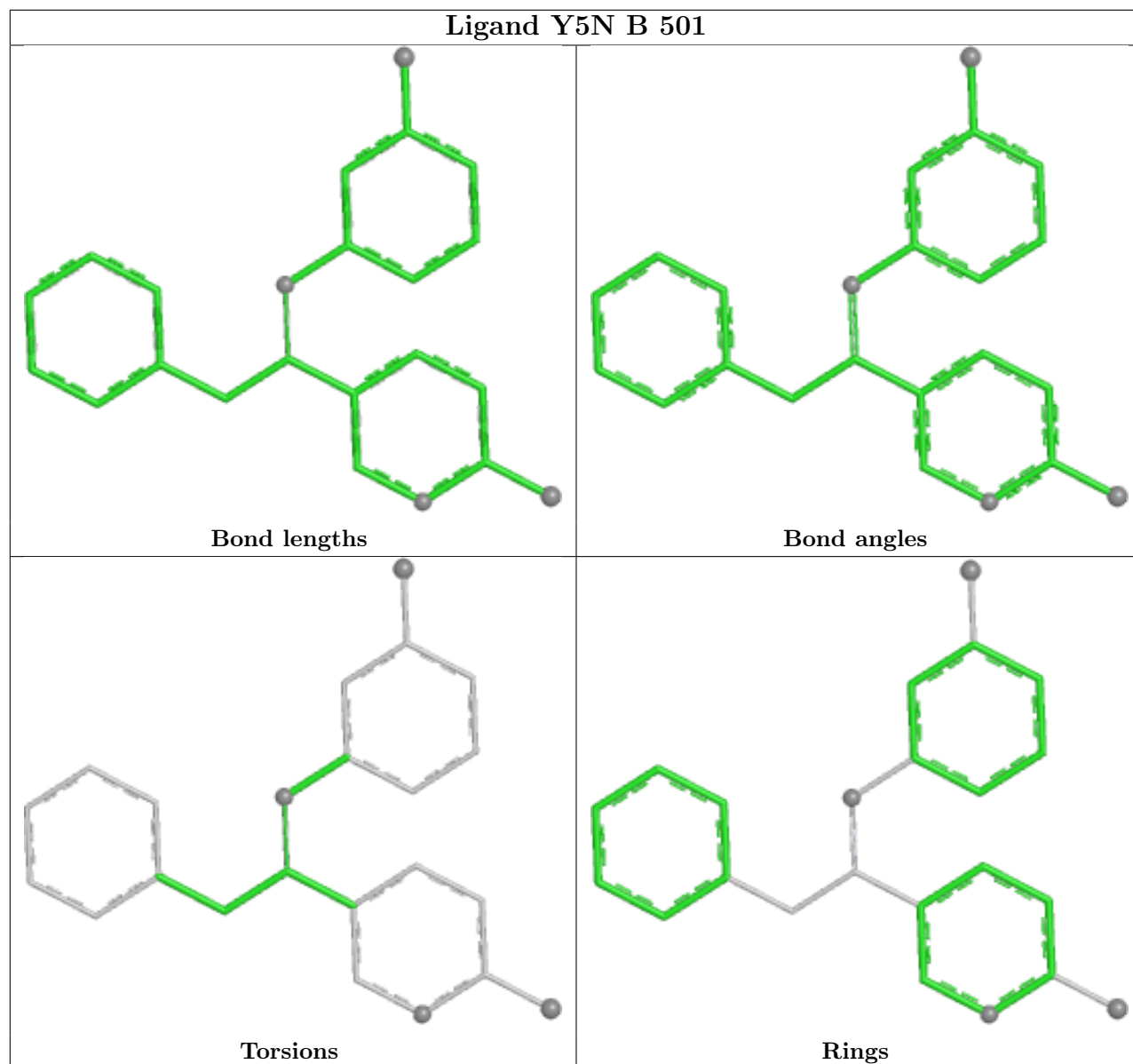


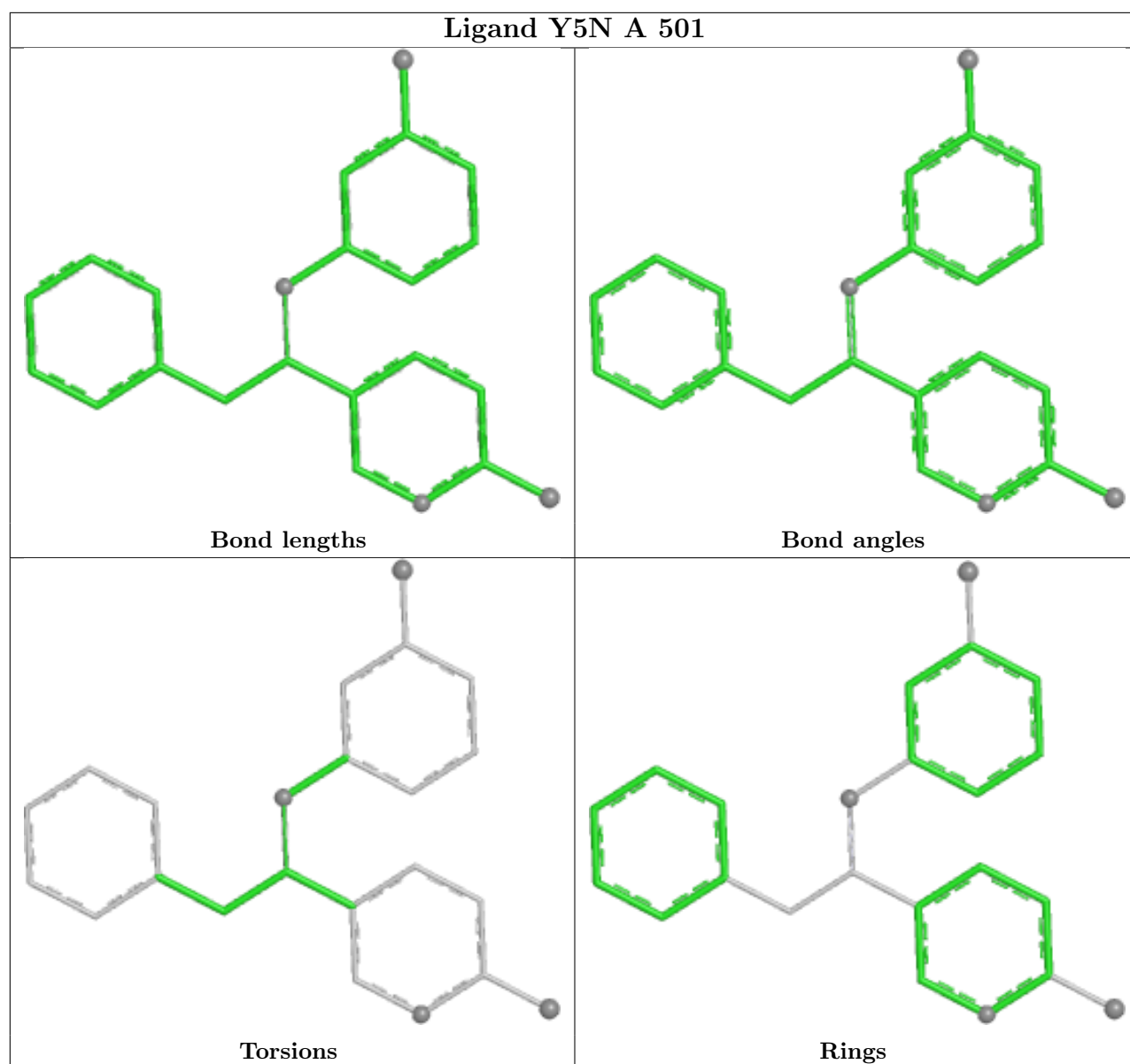
Rings

Ligand Y5N C 501



Ligand Y5N B 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

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	314/358 (87%)	-0.01	10 (3%)	50 28	50, 78, 113, 144	0
1	B	318/358 (88%)	0.05	11 (3%)	47 26	49, 77, 128, 139	0
1	C	317/358 (88%)	0.06	3 (0%)	81 61	53, 84, 119, 129	0
1	D	314/358 (87%)	0.26	5 (1%)	70 47	56, 89, 141, 159	0
All	All	1263/1432 (88%)	0.09	29 (2%)	61 38	49, 82, 126, 159	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	316	ASP	3.6
1	A	338	SER	3.1
1	A	359	TYR	3.0
1	B	187	GLU	2.9
1	A	382	ASN	2.9
1	D	356	SER	2.8
1	B	376	HIS	2.7
1	B	192	LEU	2.7
1	D	188	GLU	2.6
1	D	389	LEU	2.6
1	D	245	GLU	2.5
1	B	197	GLN	2.4
1	A	385	ILE	2.3
1	A	388	PHE	2.3
1	A	169	GLN	2.3
1	A	361	VAL	2.2
1	B	337	GLY	2.2
1	C	390	GLU	2.2
1	A	318	ASP	2.2
1	A	151	SER	2.2
1	C	249	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	329	VAL	2.1
1	B	382	ASN	2.1
1	B	242	GLN	2.1
1	B	190	GLU	2.1
1	B	385	ILE	2.1
1	B	300	GLU	2.1
1	C	389	LEU	2.0
1	D	246	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

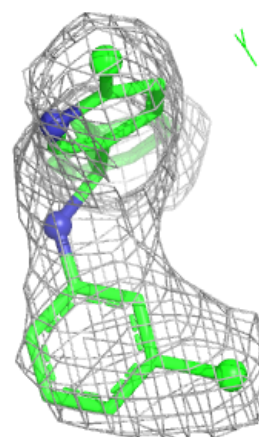
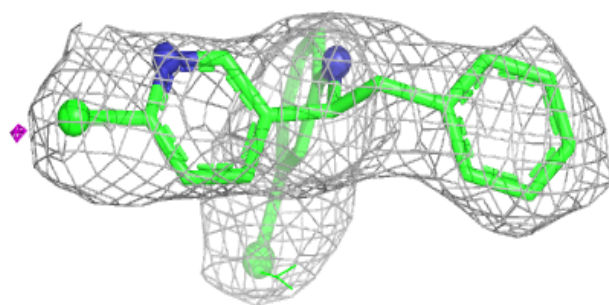
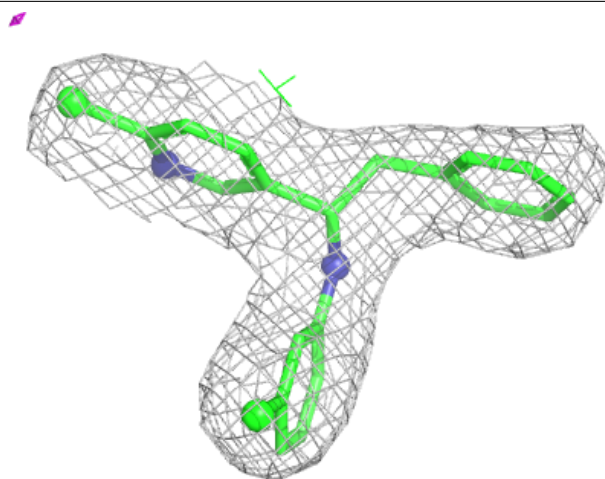
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	ZIQ	A	502	16/16	0.86	0.15	92,92,93,93	0
2	Y5N	D	501	23/23	0.90	0.13	86,88,88,88	0
2	Y5N	B	501	23/23	0.92	0.12	75,75,80,81	0
2	Y5N	C	501	23/23	0.92	0.12	87,88,89,90	0
3	ZIQ	D	502	16/16	0.92	0.10	88,89,90,90	0
2	Y5N	A	501	23/23	0.93	0.10	71,72,77,79	0
3	ZIQ	C	502	16/16	0.94	0.09	79,79,80,80	0
3	ZIQ	B	502	16/16	0.96	0.07	71,71,72,72	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.

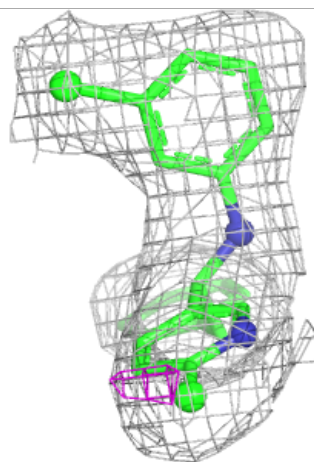
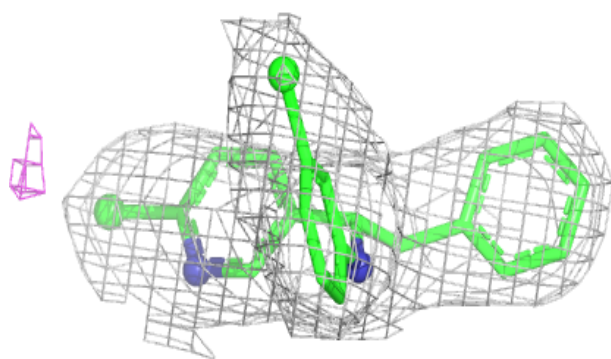
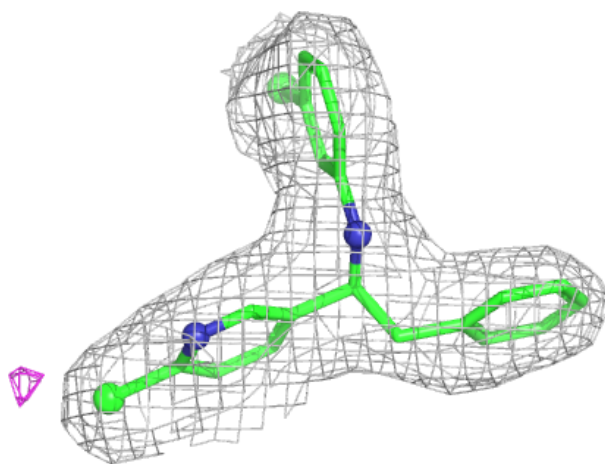
Electron density around Y5N D 501:

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



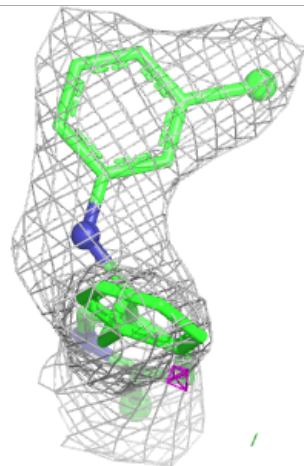
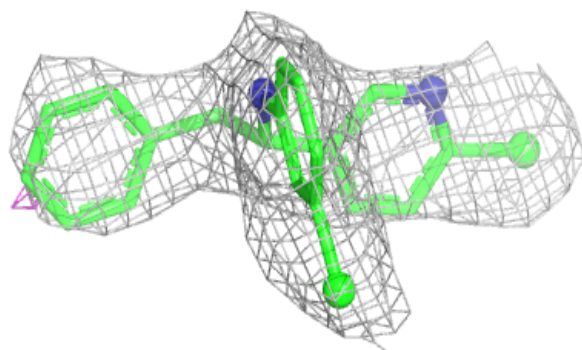
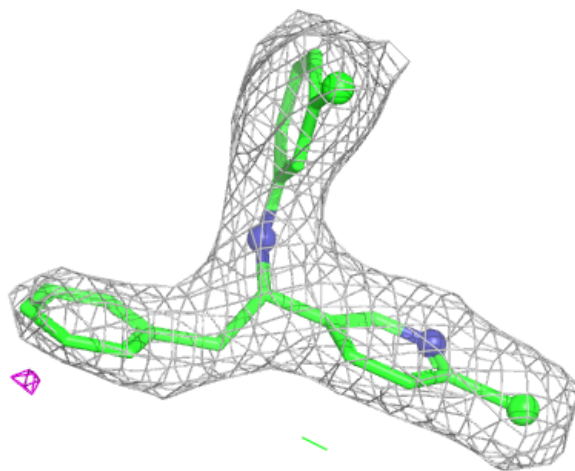
Electron density around Y5N B 501:

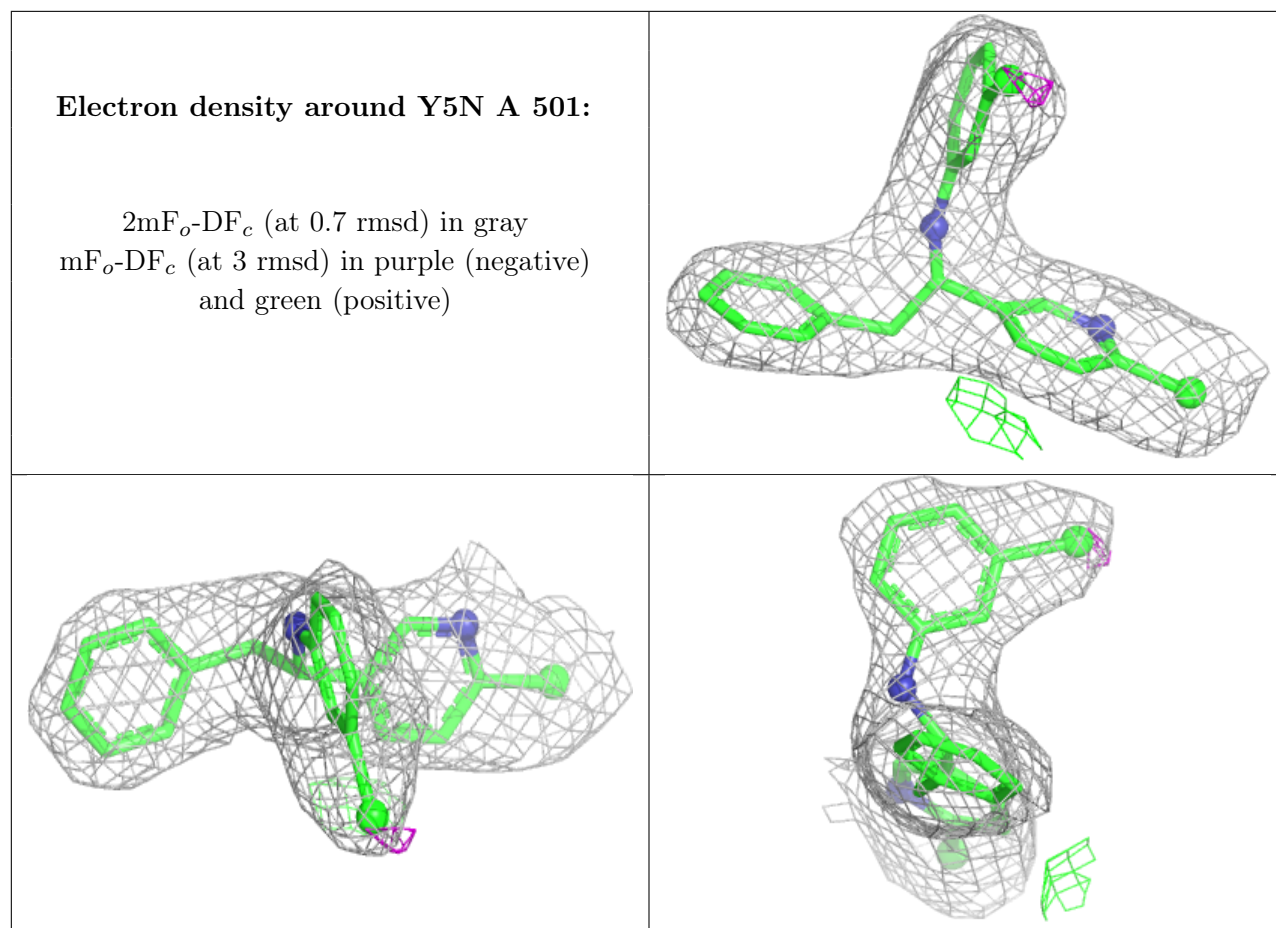
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Y5N 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.