



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 09:50 PM EDT

PDB ID : 7LK1  
Title : Ornithine Aminotransferase (OAT) with its potent inhibitor - (S)-3-amino-4,4-difluorocyclopent-1-enecarboxylic acid (SS-1-148) - 1 Hour Soaking  
Authors : Butrin, A.; Shen, S.; Liu, D.; Silverman, R.  
Deposited on : 2021-02-01  
Resolution : 1.79 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

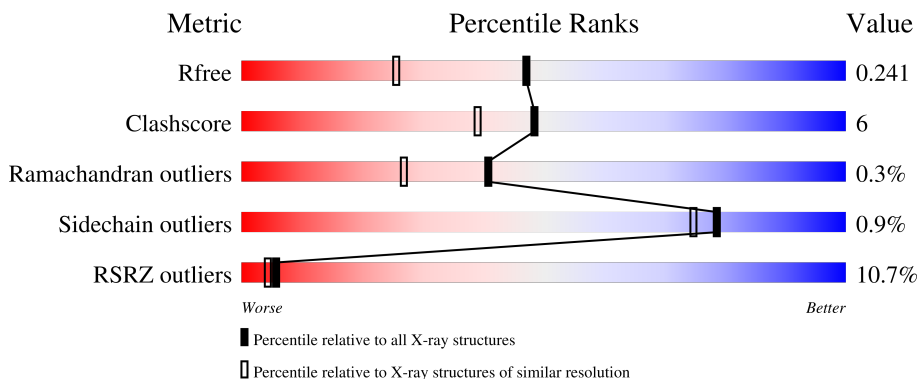
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	404	 17% 82% 1% 1%
1	B	404	 10% 85% 4% 1%
1	C	404	 5% 91% 4% 1%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	Y37	A	501[B]	X	-	-	-
2	Y37	C	501[A]	X	-	-	-
2	Y37	C	501[B]	X	-	-	-

## 2 Entry composition [i](#)

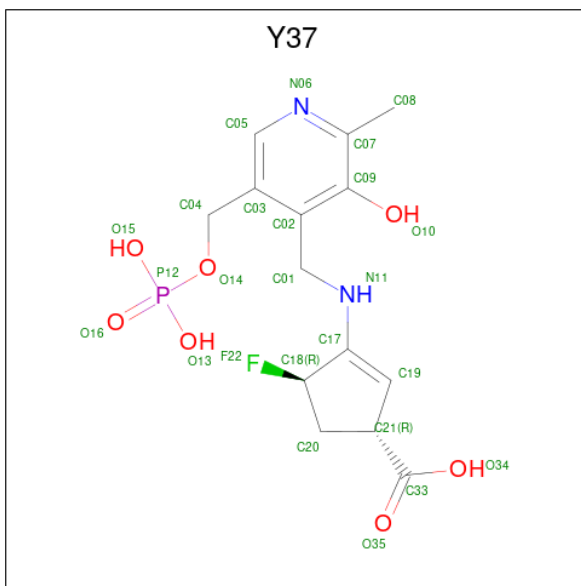
There are 3 unique types of molecules in this entry. The entry contains 10380 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ornithine aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	404	Total 3166	C 2034	N 535	O 585	S 12	0	1	0
1	B	403	Total 3157	C 2028	N 532	O 585	S 12	0	0	0
1	C	404	Total 3166	C 2034	N 535	O 585	S 12	0	1	0

- Molecule 2 is (1R,4R)-4-fluoro-3-[(3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methyl]amino)cyclopent-2-ene-1-carboxylic acid (three-letter code: Y37) (formula: C<sub>14</sub>H<sub>18</sub>FN<sub>2</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	P		
2	A	1	Total 50	C 28	F 2	N 4	O 14	P 2	0	1
2	B	1	Total 25	C 14	F 1	N 2	O 7	P 1	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	P		
2	C	1	50	28	2	4	14	2	0	1

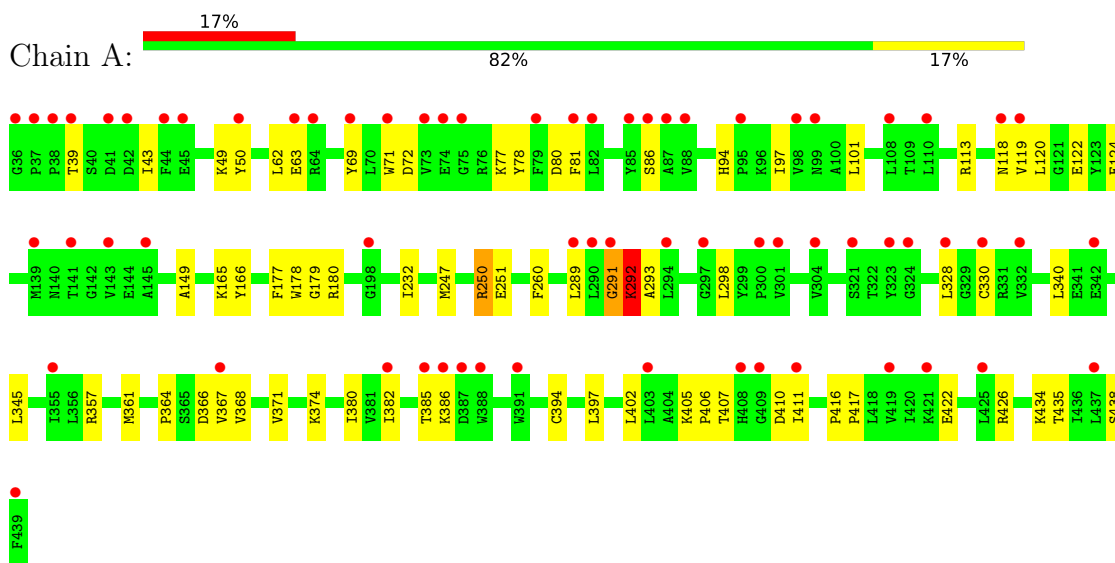
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	243	243	243	0	0
3	B	224	224	224	0	0
3	C	299	299	299	0	0

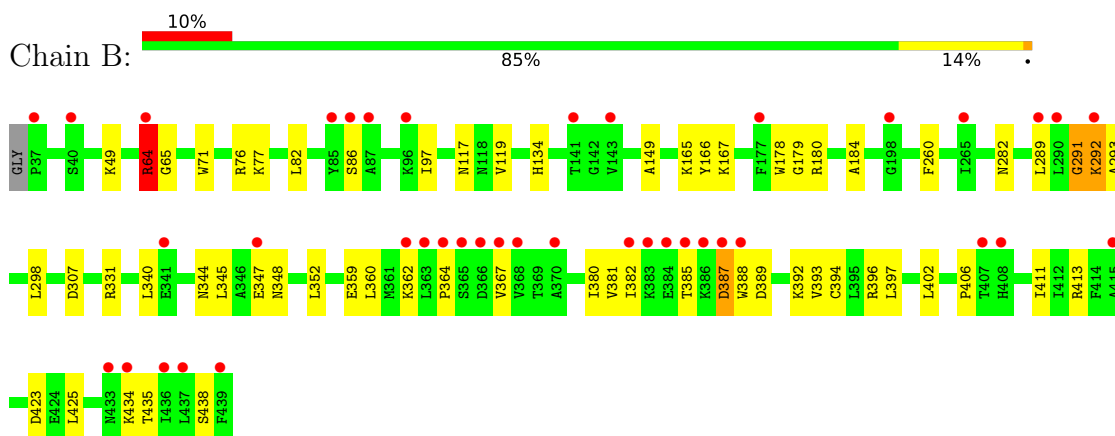
### 3 Residue-property plots

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.

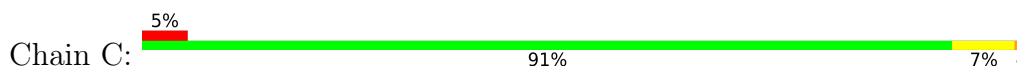
- Molecule 1: Ornithine aminotransferase, mitochondrial

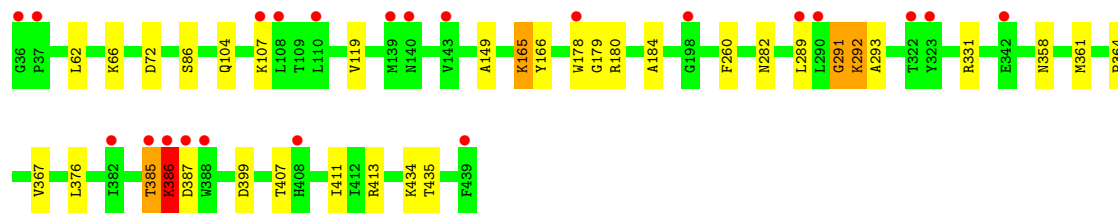


- Molecule 1: Ornithine aminotransferase, mitochondrial



- Molecule 1: Ornithine aminotransferase, mitochondrial





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.65Å 115.65Å 186.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.32 – 1.79 36.32 – 1.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.32-1.79) 100.0 (36.32-1.79)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 1.79Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.216 , 0.241 0.216 , 0.241	Depositor DCC
$R_{free}$ test set	6743 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtrriage
Anisotropy	0.087	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10380	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: Y37

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	0.37	0/3240	0.63	7/4399 (0.2%)
1	B	0.34	0/3231	0.84	4/4387 (0.1%)
1	C	0.36	0/3240	0.59	2/4399 (0.0%)
All	All	0.36	0/9711	0.69	13/13185 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
1	C	0	5
All	All	0	12

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	GLY	O-C-N	-41.07	56.99	122.70
1	A	292[A]	LYS	O-C-N	-11.76	103.89	122.70
1	A	292[B]	LYS	O-C-N	-11.76	103.89	122.70
1	C	291	GLY	O-C-N	-10.39	106.07	122.70
1	B	64	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	B	292	LYS	O-C-N	-7.63	110.49	122.70
1	A	250	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	C	291	GLY	CA-C-N	-6.29	103.36	117.20
1	A	291	GLY	C-N-CA	6.13	137.03	121.70
1	B	64	ARG	CD-NE-CZ	6.11	132.16	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	292[A]	LYS	CA-C-N	5.16	128.55	117.20
1	A	292[B]	LYS	CA-C-N	5.16	128.55	117.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	GLY	Mainchain
1	A	292[A]	LYS	Mainchain
1	A	292[B]	LYS	Mainchain
1	B	291	GLY	Peptide,Mainchain
1	B	292	LYS	Mainchain
1	C	165	LYS	Peptide
1	C	291	GLY	Mainchain
1	C	385	THR	Peptide
1	C	386	LYS	Peptide

## 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	3166	0	3169	48	0
1	B	3157	0	3160	46	0
1	C	3166	0	3170	22	0
2	A	50	0	0	3	0
2	B	25	0	0	2	0
2	C	50	0	0	2	0
3	A	243	0	0	5	0
3	B	224	0	0	5	0
3	C	299	0	0	3	0
All	All	10380	0	9499	115	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 (115) 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:B:64:ARG:HE	1:B:65:GLY:H	1.17	0.90
1:B:64:ARG:HE	1:B:65:GLY:N	1.74	0.85
1:B:64:ARG:HB3	1:B:71:TRP:HB2	1.66	0.77
1:C:180:ARG:NH1	3:C:602:HOH:O	2.17	0.77
1:C:104:GLN:HA	1:C:107:LYS:HG2	1.67	0.74
1:B:64:ARG:HH21	1:B:65:GLY:H	1.35	0.73
1:A:397:LEU:HD22	1:A:402:LEU:HD22	1.71	0.73
1:B:167:LYS:HE3	3:B:601:HOH:O	1.88	0.72
1:B:64:ARG:NE	1:B:65:GLY:H	1.88	0.71
1:B:117:ASN:ND2	3:B:602:HOH:O	2.25	0.70
1:A:78:TYR:OH	3:A:601:HOH:O	2.10	0.70
1:B:397:LEU:HD22	1:B:435:THR:HG21	1.74	0.70
1:C:165:LYS:NZ	3:C:603:HOH:O	2.22	0.69
1:A:180:ARG:NH1	3:A:603:HOH:O	2.25	0.67
1:B:413:ARG:NH1	2:B:501:Y37:O35	2.28	0.66
1:A:250:ARG:O	1:A:250:ARG:HD3	1.95	0.66
1:A:49:LYS:HD3	1:A:50:TYR:CZ	2.31	0.65
1:A:397:LEU:HG	1:A:435:THR:HG21	1.77	0.64
1:B:397:LEU:HD12	1:B:402:LEU:HD22	1.79	0.64
1:B:381:VAL:HG22	1:B:411:ILE:HG12	1.80	0.63
1:B:64:ARG:NH2	1:B:65:GLY:O	2.32	0.63
1:B:64:ARG:NH2	1:B:65:GLY:H	1.97	0.62
1:C:399:ASP:OD2	3:C:601:HOH:O	2.17	0.60
1:B:64:ARG:HH21	1:B:65:GLY:N	2.02	0.58
1:A:63:GLU:OE2	1:A:63:GLU:HA	2.04	0.57
1:C:62:LEU:HA	1:C:72:ASP:HA	1.86	0.57
1:B:394:CYS:SG	1:B:406:PRO:HD3	2.45	0.57
1:C:292[B]:LYS:NZ	2:C:501[B]:Y37:O10	2.39	0.55
1:A:122:GLU:OE1	3:A:602:HOH:O	2.17	0.55
1:B:49:LYS:NZ	3:B:605:HOH:O	2.38	0.55
1:B:180:ARG:NH1	3:B:603:HOH:O	2.37	0.55
1:C:104:GLN:NE2	1:C:107:LYS:HG3	2.22	0.54
1:B:364:PRO:HG2	1:B:367:VAL:HG22	1.90	0.53
1:A:394:CYS:SG	1:A:406:PRO:HD3	2.48	0.53
1:B:64:ARG:NH1	3:B:607:HOH:O	2.41	0.53
1:A:364:PRO:HG2	1:A:367:VAL:HG22	1.91	0.53
1:B:282:ASN:HB3	1:C:282:ASN:HB3	1.92	0.52
1:C:149:ALA:HB2	1:C:289:LEU:HD21	1.92	0.52
1:A:405:LYS:HG3	1:A:406:PRO:HD2	1.92	0.52
1:A:101:LEU:HD12	1:A:328:LEU:HD11	1.92	0.51
1:C:364:PRO:HG2	1:C:367:VAL:HG12	1.91	0.51
1:B:382:ILE:HD13	1:B:393:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ARG:NH2	2:C:501[B]:Y37:O34	2.38	0.51
1:A:118:ASN:OD1	1:A:119:VAL:HG23	2.10	0.51
1:A:434:LYS:O	1:A:438:SER:OG	2.23	0.51
1:A:340:LEU:HD23	1:A:345:LEU:HD12	1.93	0.51
1:B:149:ALA:HB2	1:B:289:LEU:HD21	1.93	0.50
1:A:292[A]:LYS:NZ	2:A:501[A]:Y37:O10	2.45	0.50
1:A:118:ASN:OD1	1:A:118:ASN:N	2.45	0.50
1:A:385:THR:OG1	1:A:386:LYS:N	2.44	0.50
1:A:149:ALA:HB2	1:A:289:LEU:HD21	1.94	0.49
1:A:250:ARG:HD3	1:A:250:ARG:C	2.31	0.49
1:B:86:SER:O	1:B:293:ALA:HB2	2.12	0.49
1:A:62:LEU:HA	1:A:72:ASP:HA	1.94	0.49
1:A:371:VAL:HG22	1:A:380:ILE:HG22	1.95	0.48
1:C:407:THR:OG1	1:C:411:ILE:HB	2.14	0.48
1:A:367:VAL:HG23	1:A:368:VAL:HG23	1.95	0.48
1:B:71:TRP:HA	1:B:76:ARG:O	2.14	0.47
1:A:94:HIS:HB3	1:A:97:ILE:HD12	1.96	0.47
1:B:352:LEU:HB3	1:B:425:LEU:HD22	1.96	0.47
1:C:179:GLY:C	1:C:180:ARG:HD2	2.35	0.47
1:A:422:GLU:O	1:A:426:ARG:HG3	2.15	0.47
1:B:396:ARG:HH11	1:B:438:SER:HB2	1.80	0.47
1:B:360:LEU:HD22	1:B:380:ILE:HG21	1.97	0.46
1:C:86:SER:O	1:C:293:ALA:HB2	2.16	0.46
1:A:119:VAL:HG12	1:A:330:CYS:HB3	1.97	0.46
1:A:178:TRP:HA	2:A:501[B]:Y37:C05	2.45	0.46
1:A:357:ARG:O	1:A:361:MET:HG3	2.16	0.46
1:A:232:ILE:HD11	1:A:374:LYS:HD3	1.98	0.45
1:C:178:TRP:CZ2	1:C:184:ALA:HA	2.51	0.45
1:B:119:VAL:HG11	1:B:331:ARG:HG2	1.98	0.45
1:B:389:ASP:OD2	1:B:392:LYS:HE2	2.17	0.45
1:B:64:ARG:CZ	1:B:65:GLY:H	2.27	0.45
1:B:178:TRP:CZ2	1:B:184:ALA:HA	2.52	0.45
1:B:178:TRP:HA	2:B:501:Y37:C05	2.46	0.45
1:B:165:LYS:HA	1:B:166:TYR:HA	1.71	0.44
1:C:434:LYS:HG3	1:C:435:THR:N	2.33	0.44
1:B:344:ASN:HB3	1:B:347:GLU:HG2	1.99	0.44
1:C:385:THR:OG1	1:C:386:LYS:N	2.49	0.44
1:B:396:ARG:HG2	1:B:435:THR:HG23	2.00	0.44
1:A:178:TRP:HA	2:A:501[A]:Y37:C05	2.47	0.43
1:A:250:ARG:HD2	3:A:641:HOH:O	2.18	0.43
1:B:359:GLU:HA	1:B:362:LYS:HZ2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:TRP:NE1	1:A:77:LYS:HG3	2.33	0.43
1:B:134:HIS:HB2	1:B:307:ASP:HA	2.00	0.43
1:A:382:ILE:N	1:A:410:ASP:O	2.37	0.43
1:A:179:GLY:C	1:A:180:ARG:HD2	2.39	0.42
1:A:86:SER:O	1:A:293:ALA:HB2	2.19	0.42
1:C:104:GLN:CD	1:C:107:LYS:HG3	2.40	0.42
1:A:97:ILE:HG22	1:A:298:LEU:HD22	2.02	0.42
1:A:177:PHE:CZ	1:A:180:ARG:HD3	2.54	0.42
1:C:358:ASN:HA	1:C:361:MET:HE3	2.01	0.42
1:A:165:LYS:HA	1:A:166:TYR:HA	1.77	0.42
1:B:340:LEU:HD23	1:B:345:LEU:HD12	2.02	0.42
1:B:77:LYS:HE3	1:B:77:LYS:HB3	1.79	0.42
1:C:119:VAL:HG11	1:C:331:ARG:HG2	2.02	0.42
1:B:434:LYS:O	1:B:438:SER:OG	2.35	0.42
1:A:247:MET:O	1:A:251:GLU:HG3	2.20	0.41
1:A:179:GLY:O	1:A:180:ARG:HD2	2.20	0.41
1:A:69:TYR:CG	1:A:77:LYS:HE2	2.55	0.41
1:B:64:ARG:NE	1:B:64:ARG:HA	2.36	0.41
1:B:385:THR:C	1:B:387:ASP:H	2.24	0.41
1:A:39:THR:O	1:A:43:ILE:HG13	2.21	0.41
1:A:81:PHE:CE1	1:A:416:PRO:HB3	2.54	0.41
1:A:407:THR:HG22	1:A:411:ILE:HB	2.02	0.41
1:A:113:ARG:HD2	3:A:703:HOH:O	2.20	0.41
1:A:80:ASP:O	1:A:417:PRO:HD3	2.21	0.40
1:A:120:LEU:O	1:A:124:GLU:HG3	2.21	0.40
1:B:179:GLY:O	1:B:180:ARG:HD2	2.21	0.40
1:A:71:TRP:CZ2	1:A:77:LYS:HE3	2.56	0.40
1:B:97:ILE:HG22	1:B:298:LEU:HD22	2.02	0.40
1:C:66:LYS:HD3	1:C:66:LYS:HA	1.83	0.40
1:C:376:LEU:HD23	1:C:376:LEU:HA	1.93	0.40
1:B:423:ASP:OD1	1:B:423:ASP:N	2.55	0.40
1:B:347:GLU:HG3	1:B:348:ASN:N	2.36	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	403/404 (100%)	380 (94%)	21 (5%)	2 (0%)	29	15
1	B	401/404 (99%)	380 (95%)	21 (5%)	0	100	100
1	C	403/404 (100%)	381 (94%)	18 (4%)	4 (1%)	15	5
All	All	1207/1212 (100%)	1141 (94%)	60 (5%)	6 (0%)	41	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292[A]	LYS
1	A	292[B]	LYS
1	C	166	TYR
1	C	292[A]	LYS
1	C	292[B]	LYS
1	C	386	LYS

### 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	337/337 (100%)	335 (99%)	2 (1%)	86	84
1	B	337/337 (100%)	332 (98%)	5 (2%)	65	56
1	C	337/337 (100%)	335 (99%)	2 (1%)	86	84
All	All	1011/1011 (100%)	1002 (99%)	9 (1%)	78	75

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	PHE
1	A	366	ASP
1	B	64	ARG

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Mol	Chain	Res	Type
1	B	82	LEU
1	B	260	PHE
1	B	387	ASP
1	B	388	TRP
1	C	260	PHE
1	C	387	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	344	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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	Y37	C	501[B]	1	23,26,26	1.99	1 (4%)	26,38,38	1.75	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	Y37	C	501[A]	1	23,26,26	1.97	1 (4%)	26,38,38	2.02	6 (23%)
2	Y37	B	501	1	23,26,26	1.86	1 (4%)	26,38,38	1.80	2 (7%)
2	Y37	A	501[B]	1	23,26,26	2.10	1 (4%)	26,38,38	1.66	3 (11%)
2	Y37	A	501[A]	1	23,26,26	1.94	2 (8%)	26,38,38	1.92	3 (11%)

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	Y37	C	501[B]	1	1/1/5/7	0/14/27/27	0/2/2/2
2	Y37	C	501[A]	1	2/2/5/7	0/14/27/27	0/2/2/2
2	Y37	B	501	1	-	4/14/27/27	0/2/2/2
2	Y37	A	501[B]	1	2/2/5/7	3/14/27/27	0/2/2/2
2	Y37	A	501[A]	1	-	1/14/27/27	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[B]	Y37	C17-N11	8.55	1.45	1.34
2	C	501[B]	Y37	C17-N11	8.10	1.45	1.34
2	C	501[A]	Y37	C17-N11	7.93	1.45	1.34
2	A	501[A]	Y37	C17-N11	7.64	1.44	1.34
2	B	501	Y37	C17-N11	6.97	1.43	1.34
2	A	501[A]	Y37	C09-C07	-2.41	1.38	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501[A]	Y37	F22-C18-C20	7.81	120.86	109.53
2	B	501	Y37	F22-C18-C20	7.72	120.72	109.53
2	A	501[A]	Y37	F22-C18-C20	7.55	120.49	109.53
2	C	501[B]	Y37	F22-C18-C20	7.27	120.07	109.53
2	A	501[B]	Y37	F22-C18-C20	6.82	119.42	109.53
2	A	501[A]	Y37	C20-C21-C19	3.26	109.64	98.69
2	C	501[A]	Y37	C01-C02-C03	3.15	123.21	119.71
2	C	501[A]	Y37	C20-C21-C19	2.89	108.41	98.69
2	B	501	Y37	C20-C21-C19	2.72	107.81	98.69
2	A	501[B]	Y37	C20-C21-C19	2.59	107.37	98.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501[B]	Y37	C20-C21-C19	2.45	106.90	98.69
2	C	501[A]	Y37	C01-C02-C09	-2.42	117.46	120.04
2	A	501[B]	Y37	O34-C33-O35	-2.32	118.83	124.09
2	A	501[A]	Y37	C02-C01-N11	-2.20	106.73	111.22
2	C	501[A]	Y37	O34-C33-O35	-2.16	119.19	124.09
2	C	501[A]	Y37	O10-C09-C07	2.02	121.89	117.49

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501[B]	Y37	C21
2	A	501[B]	Y37	C18
2	C	501[A]	Y37	C21
2	C	501[A]	Y37	C18
2	C	501[B]	Y37	C21

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501[A]	Y37	C18-C17-N11-C01
2	B	501	Y37	C18-C17-N11-C01
2	A	501[B]	Y37	N11-C01-C02-C03
2	B	501	Y37	N11-C01-C02-C03
2	A	501[B]	Y37	N11-C01-C02-C09
2	B	501	Y37	N11-C01-C02-C09
2	A	501[B]	Y37	C19-C21-C33-O35
2	B	501	Y37	C19-C21-C33-O35

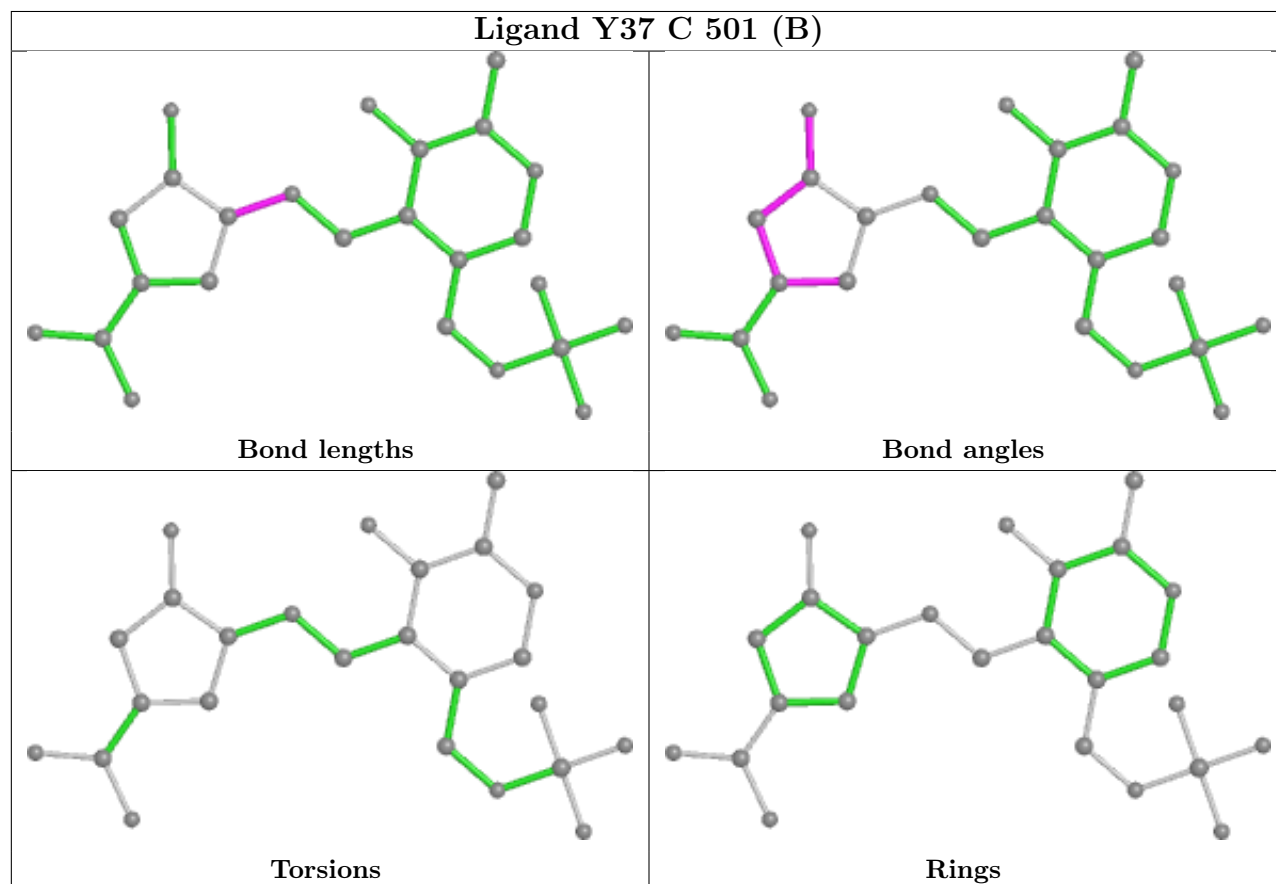
There are no ring outliers.

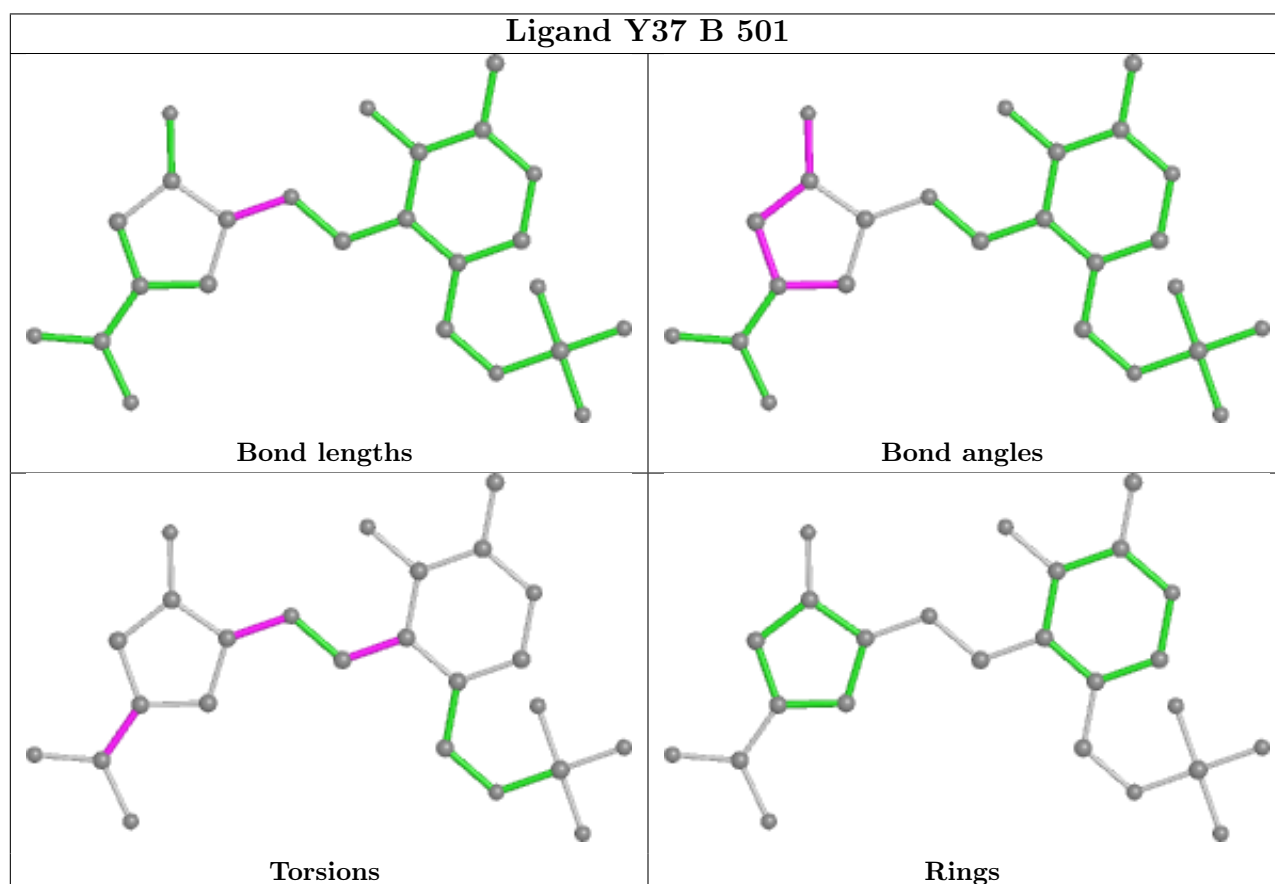
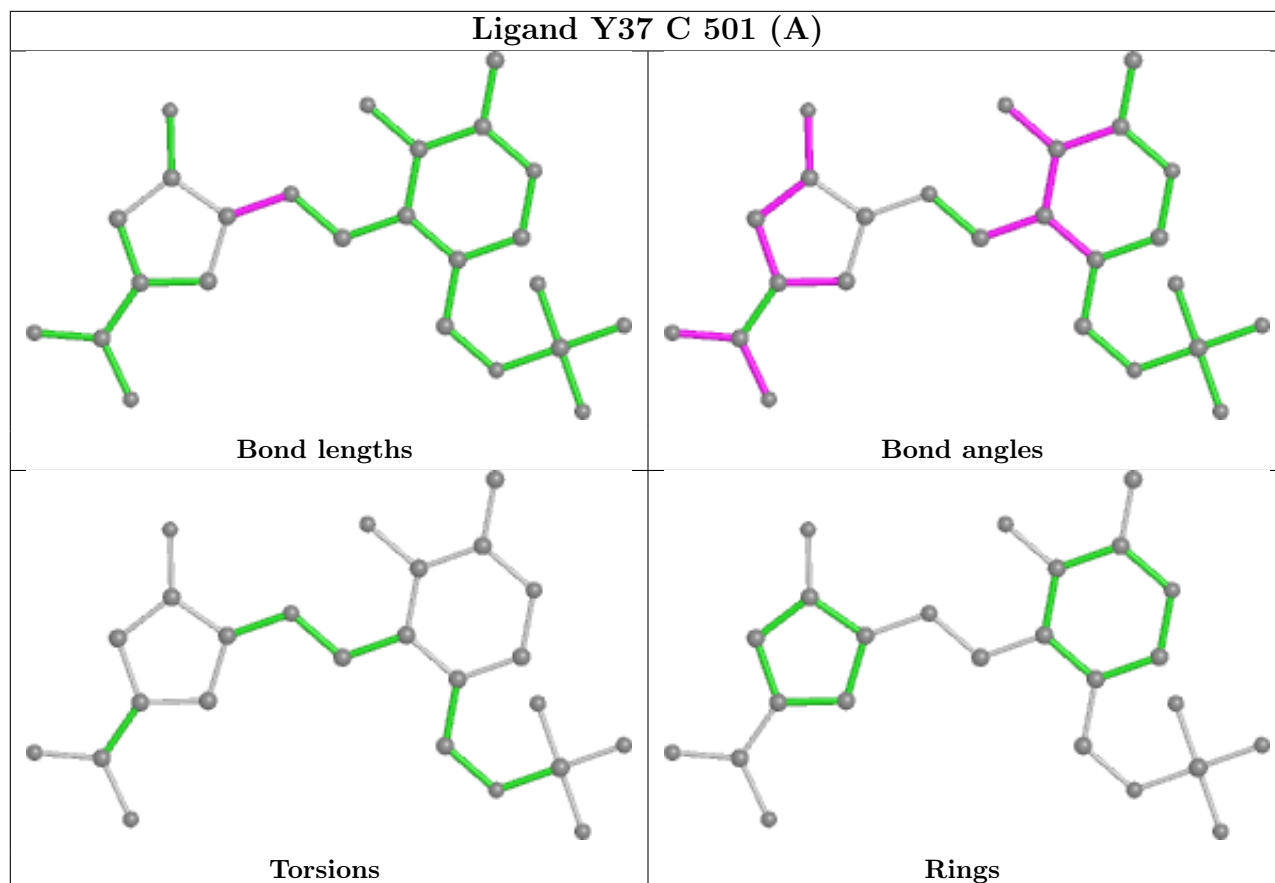
4 monomers are involved in 7 short contacts:

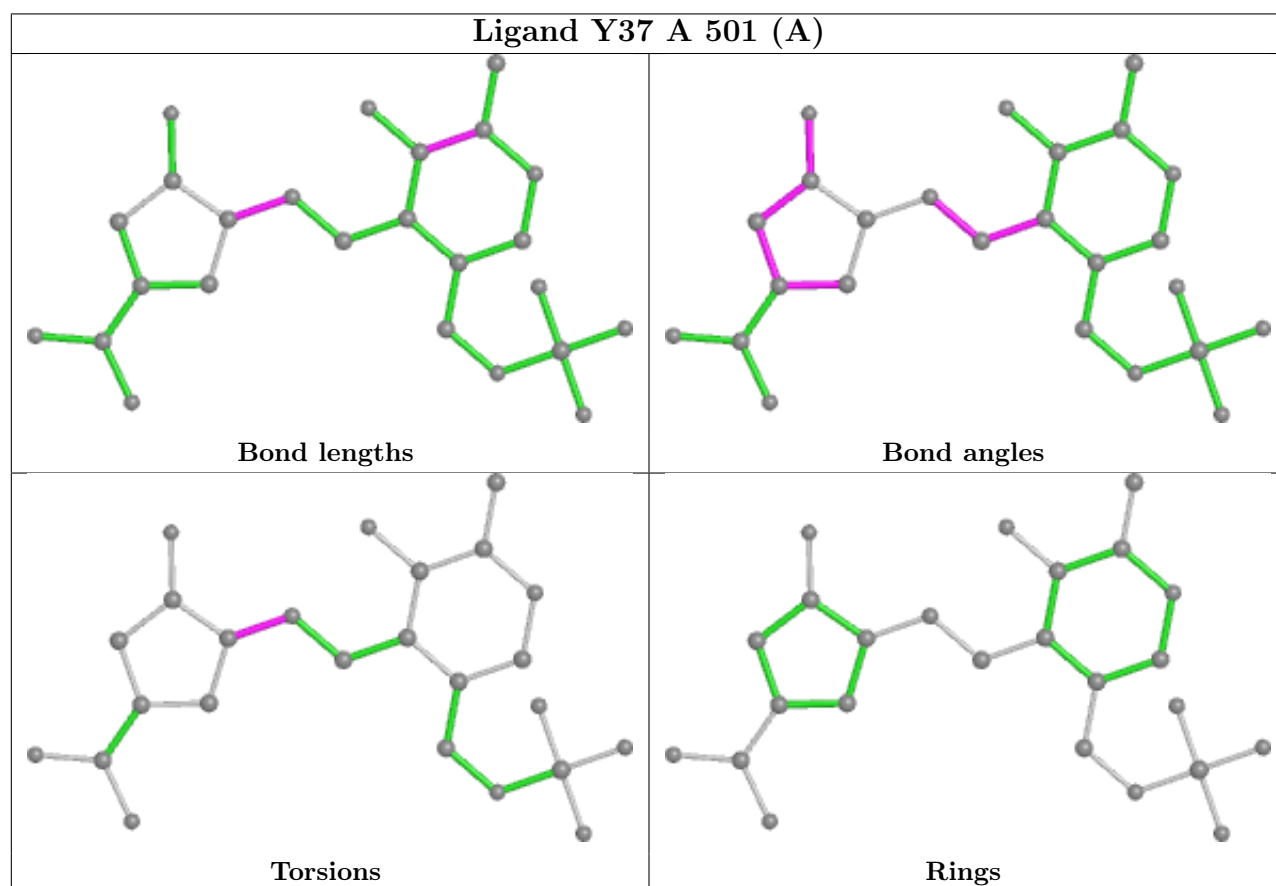
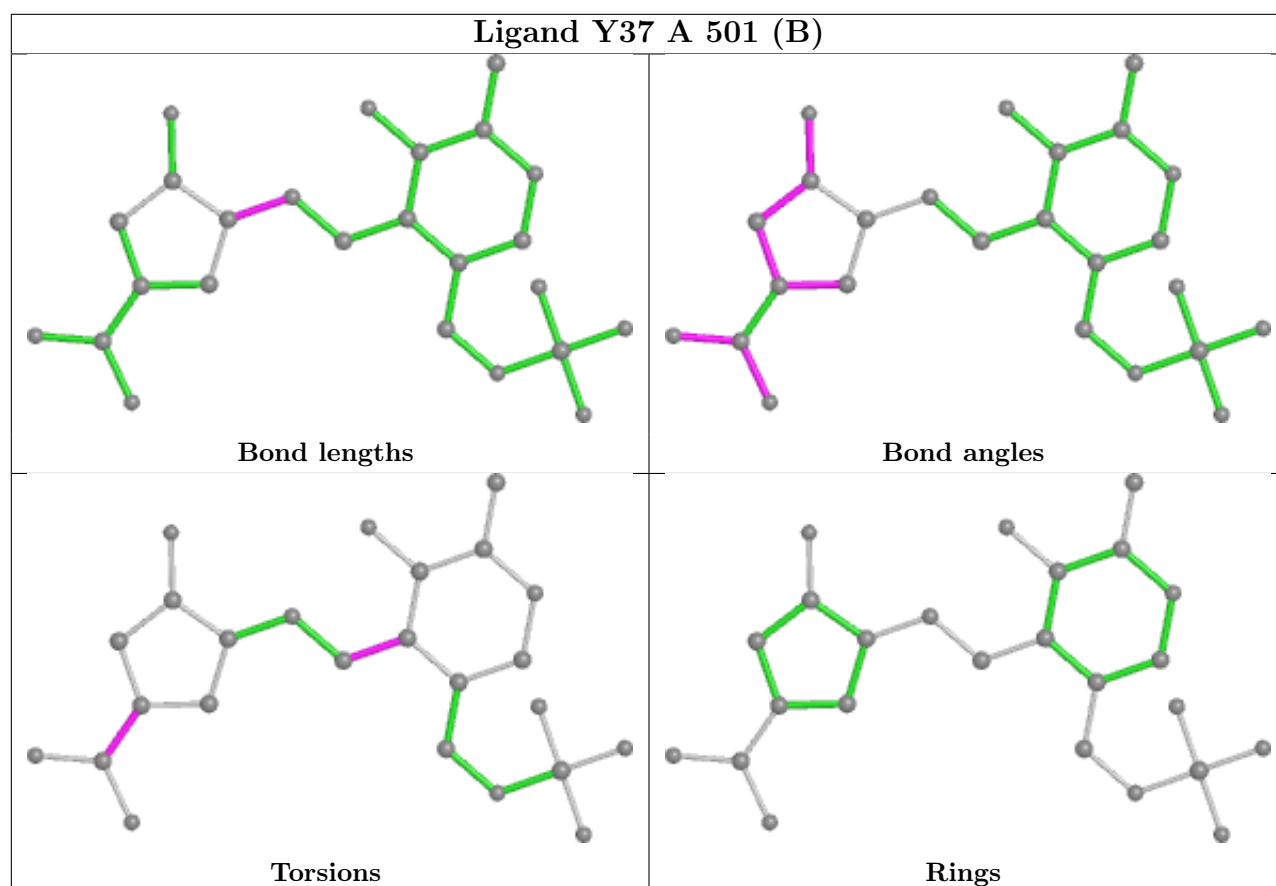
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501[B]	Y37	2	0
2	B	501	Y37	2	0
2	A	501[B]	Y37	1	0
2	A	501[A]	Y37	2	0

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 [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, 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	404/404 (100%)	0.82	67 (16%) <b>1</b> <b>1</b>	24, 45, 70, 109	0
1	B	403/404 (99%)	0.63	40 (9%) <b>7</b> <b>5</b>	25, 42, 79, 122	1 (0%)
1	C	404/404 (100%)	0.32	22 (5%) <b>25</b> <b>20</b>	25, 37, 57, 100	1 (0%)
All	All	1211/1212 (99%)	0.59	129 (10%) <b>6</b> <b>4</b>	24, 40, 72, 122	2 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	TRP	8.9
1	B	367	VAL	7.9
1	A	36	GLY	6.9
1	A	73	VAL	6.8
1	C	107	LYS	6.6
1	A	388	TRP	6.0
1	C	387	ASP	5.8
1	A	367	VAL	5.8
1	A	387	ASP	5.7
1	B	439	PHE	5.5
1	B	387	ASP	5.4
1	A	37	PRO	5.3
1	C	386	LYS	5.3
1	B	386	LYS	5.3
1	A	63	GLU	5.2
1	B	64	ARG	5.0
1	A	301	VAL	4.8
1	C	198	GLY	4.8
1	B	385	THR	4.6
1	B	437	LEU	4.5
1	A	386	LYS	4.5
1	A	198	GLY	4.4
1	A	385	THR	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	364	PRO	4.3
1	C	388	TRP	4.1
1	B	366	ASP	4.1
1	B	383	LYS	4.0
1	A	118	ASN	3.9
1	C	322	THR	3.9
1	C	385	THR	3.8
1	A	69	TYR	3.8
1	A	82	LEU	3.8
1	A	141	THR	3.7
1	A	323	TYR	3.7
1	B	384	GLU	3.7
1	B	436	ILE	3.6
1	A	39	THR	3.5
1	A	328	LEU	3.5
1	B	198	GLY	3.4
1	B	407	THR	3.4
1	B	362	LYS	3.3
1	B	37	PRO	3.3
1	A	85	TYR	3.3
1	A	44	PHE	3.2
1	B	365	SER	3.2
1	A	330	CYS	3.1
1	A	439	PHE	3.1
1	A	382	ILE	3.1
1	A	110	LEU	3.1
1	A	50	TYR	3.0
1	B	265	ILE	3.0
1	B	363	LEU	3.0
1	B	143	VAL	3.0
1	A	437	LEU	2.9
1	B	370	ALA	2.9
1	A	45	GLU	2.9
1	A	38	PRO	2.8
1	A	300	PRO	2.8
1	C	37	PRO	2.8
1	B	408	HIS	2.7
1	A	108	LEU	2.7
1	C	140	ASN	2.6
1	A	64	ARG	2.6
1	A	342	GLU	2.6
1	A	409	GLY	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	304	VAL	2.6
1	C	323	TYR	2.6
1	B	434	LYS	2.6
1	A	41	ASP	2.5
1	B	347	GLU	2.5
1	B	289	LEU	2.5
1	B	141	THR	2.5
1	B	382	ILE	2.5
1	B	415	ALA	2.5
1	A	71	TRP	2.5
1	A	425	LEU	2.5
1	A	99	ASN	2.4
1	B	433	ASN	2.4
1	A	143	VAL	2.4
1	B	40	SER	2.4
1	C	108	LEU	2.4
1	B	341	GLU	2.4
1	A	81	PHE	2.4
1	B	177	PHE	2.4
1	A	139	MET	2.4
1	A	403	LEU	2.3
1	C	110	LEU	2.3
1	B	85	TYR	2.3
1	B	87	ALA	2.3
1	C	36	GLY	2.3
1	A	290	LEU	2.3
1	C	439	PHE	2.3
1	A	95	PRO	2.3
1	C	382	ILE	2.3
1	C	408	HIS	2.3
1	A	294	LEU	2.2
1	A	355	ILE	2.2
1	A	324	GLY	2.2
1	A	419	VAL	2.2
1	C	143	VAL	2.2
1	C	342	GLU	2.2
1	A	145	ALA	2.2
1	C	178	TRP	2.2
1	A	86	SER	2.1
1	A	79	PHE	2.1
1	B	96	LYS	2.1
1	B	290	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	321	SER	2.1
1	A	42	ASP	2.1
1	A	119	VAL	2.1
1	A	289	LEU	2.1
1	A	87	ALA	2.1
1	C	289	LEU	2.1
1	C	139	MET	2.1
1	A	297	GLY	2.1
1	A	411	ILE	2.1
1	B	86	SER	2.1
1	A	88	VAL	2.1
1	B	292	LYS	2.0
1	A	74	GLU	2.0
1	A	75	GLY	2.0
1	A	332	VAL	2.0
1	B	368	VAL	2.0
1	A	391	TRP	2.0
1	A	408	HIS	2.0
1	C	290	LEU	2.0
1	A	421	LYS	2.0
1	A	98	VAL	2.0
1	A	291	GLY	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.

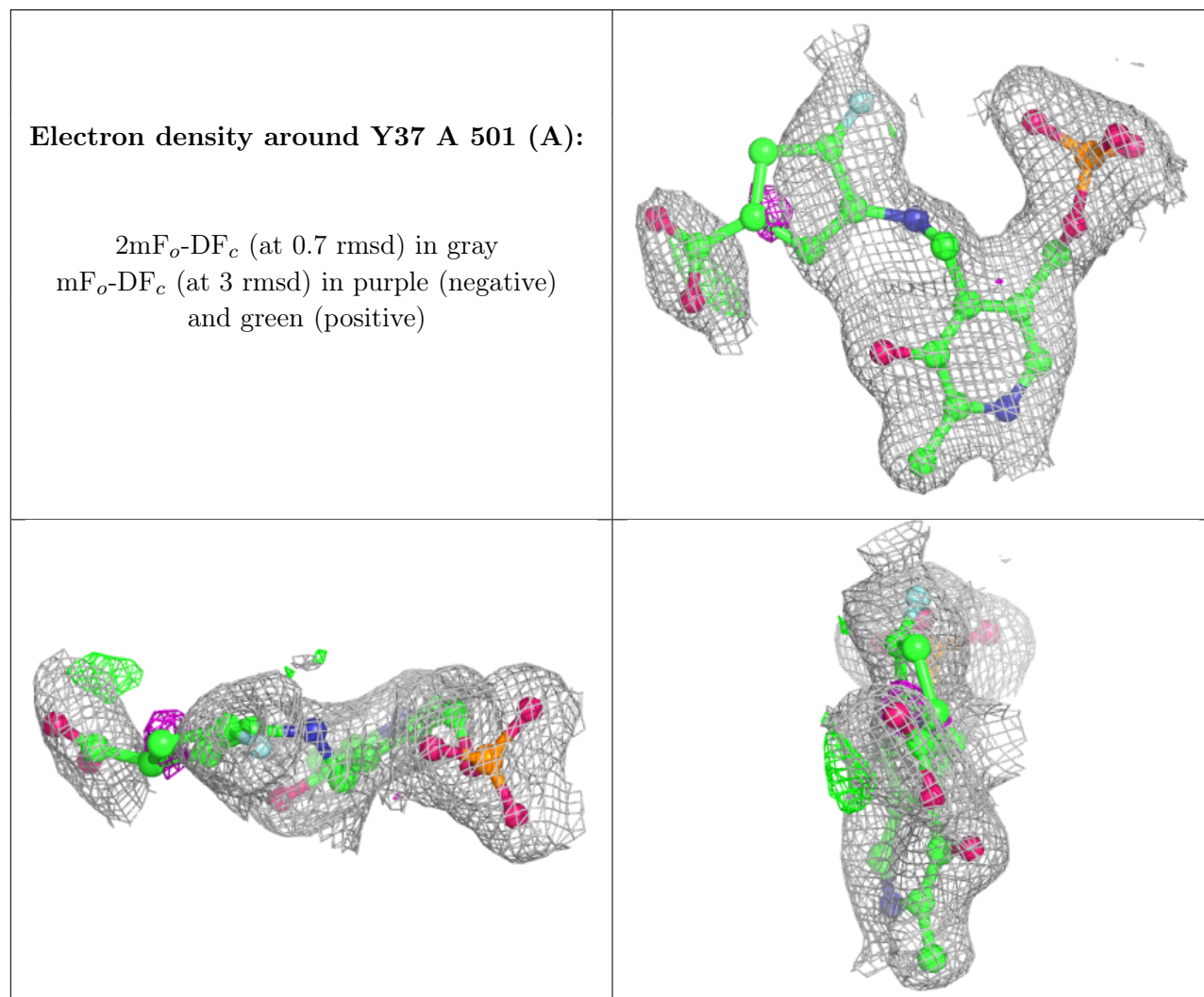
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	Y37	A	501[A]	25/25	0.95	0.21	31,40,59,66	25

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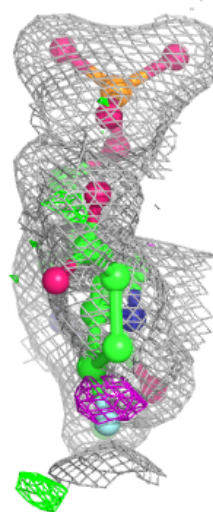
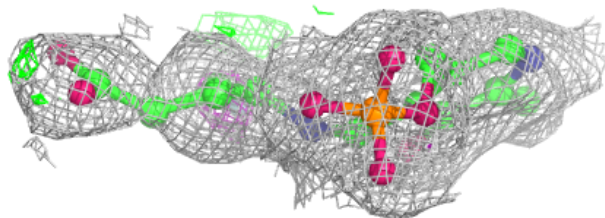
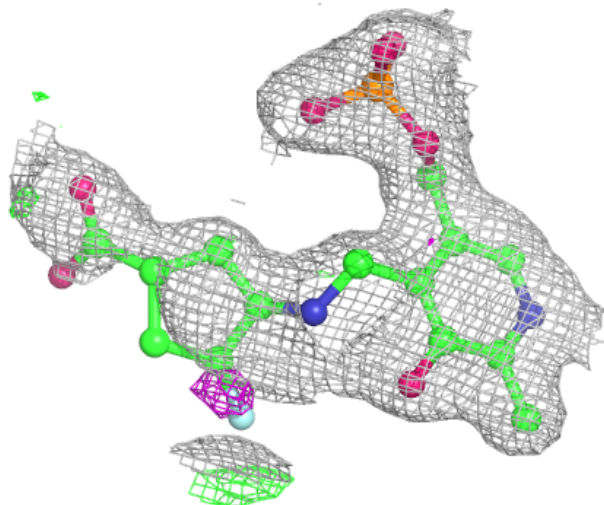
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	Y37	A	501[B]	25/25	0.95	0.21	32,38,65,78	25
2	Y37	C	501[A]	25/25	0.96	0.17	27,34,54,67	25
2	Y37	C	501[B]	25/25	0.96	0.17	28,35,61,64	25
2	Y37	B	501	25/25	0.97	0.22	30,47,80,83	0

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.



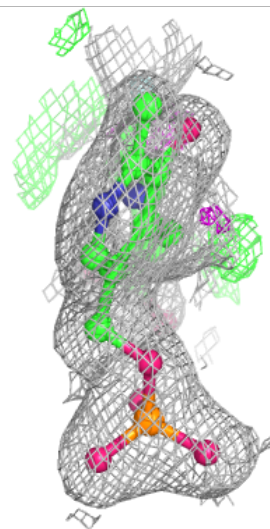
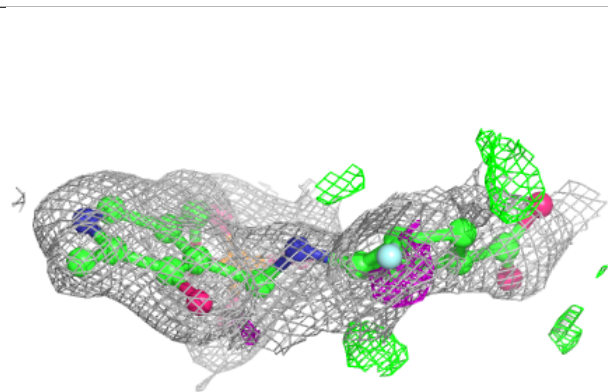
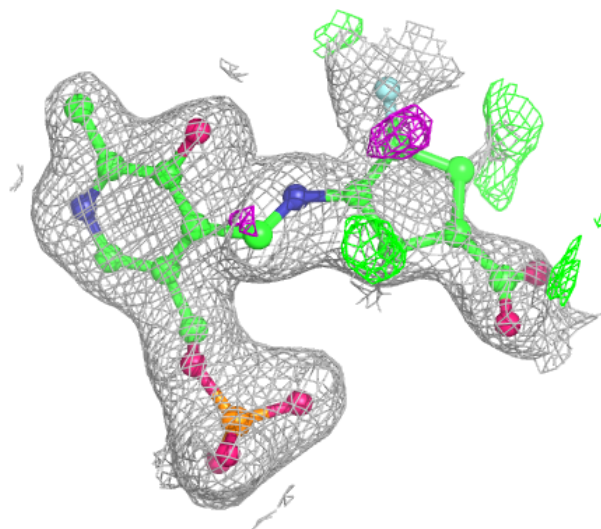
**Electron density around Y37 A 501 (B):**

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



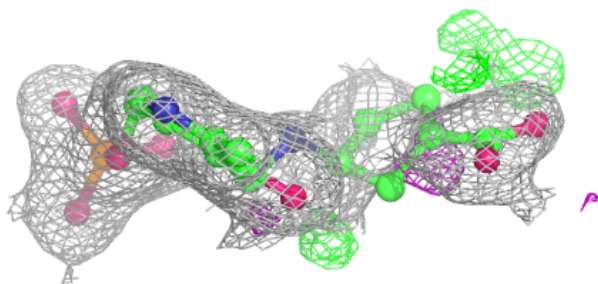
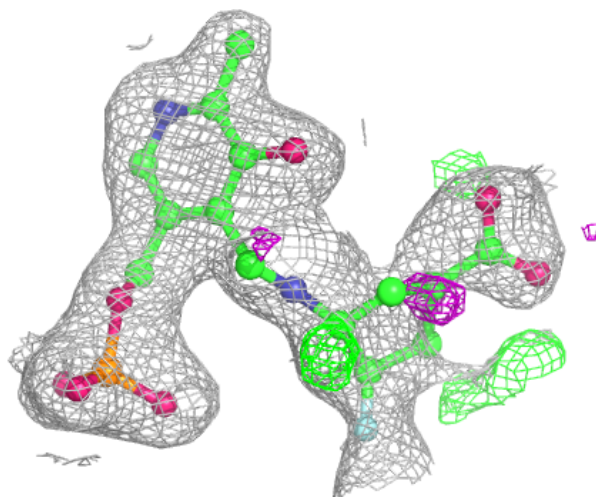
**Electron density around Y37 C 501 (A):**

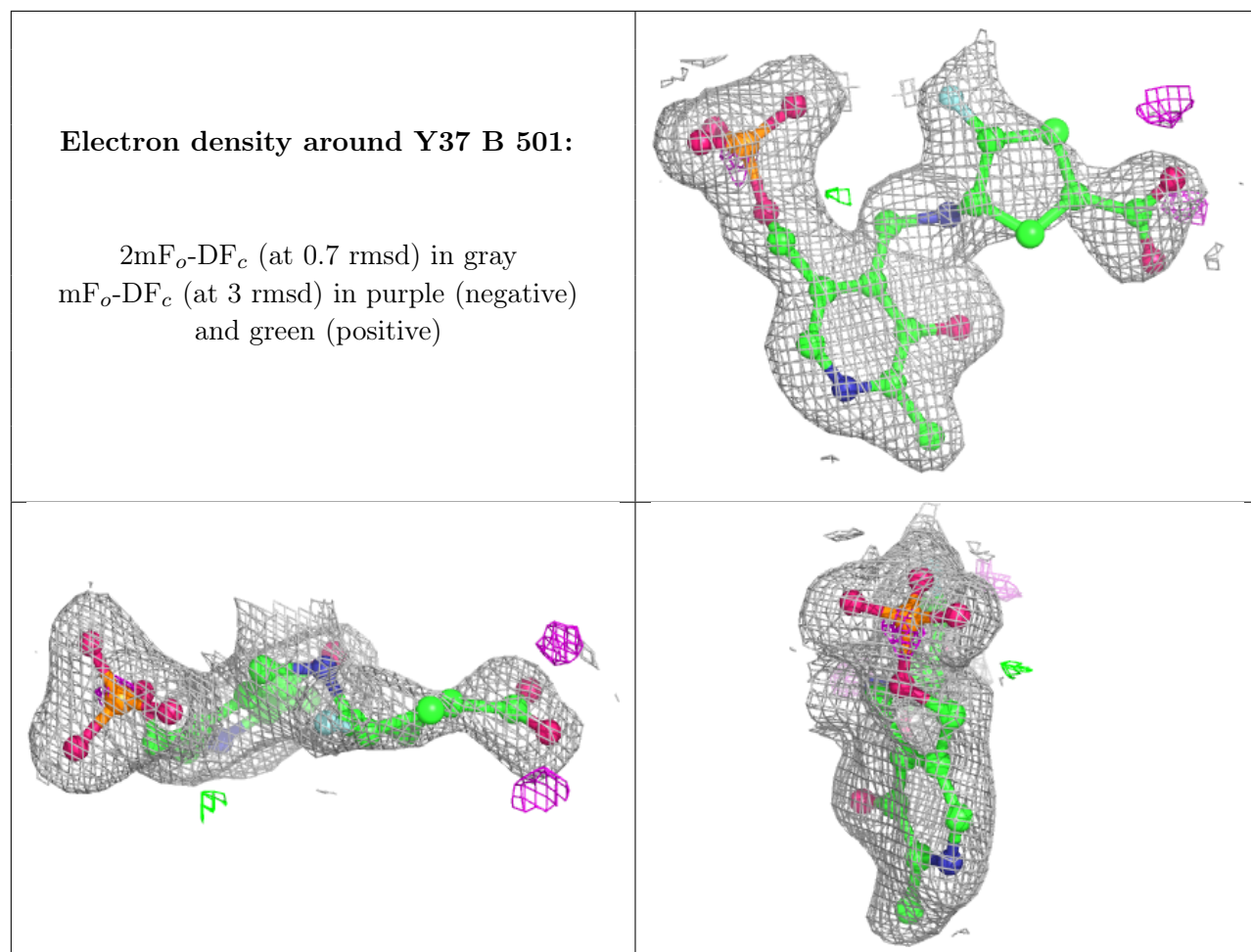
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Y37 C 501 (B):**

$2mF_o-DF_c$  (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.