



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2022 – 12:04 PM EST

PDB ID : 7LK0  
Title : Ornithine Aminotransferase (OAT) cocrystallized with its potent inhibitor - (S)-3-amino-4,4-difluorocyclopent-1-enecarboxylic acid (SS-1-148)  
Authors : Butrin, A.; Shen, S.; Liu, D.; Silverman, R.  
Deposited on : 2021-02-01  
Resolution : 1.96 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.

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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 : 2.26  
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) : 2.26

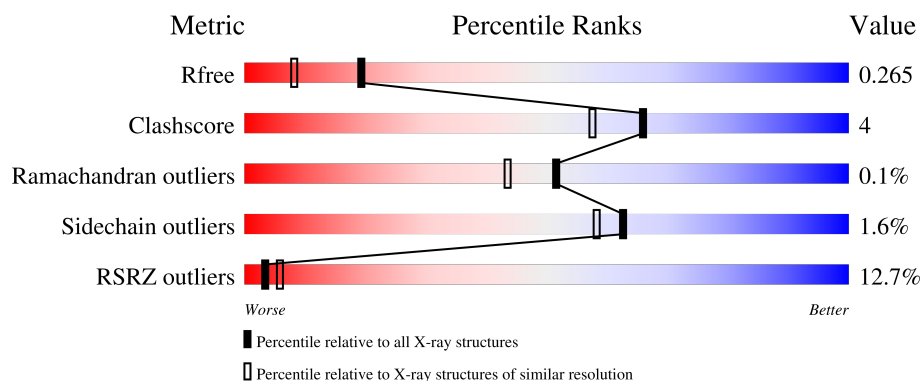
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	<div> <div>2%</div> <div>89%</div> <div>9%</div> </div>
1	B	404	<div> <div>22%</div> <div>88%</div> <div>11%</div> </div>
1	C	404	<div> <div>14%</div> <div>89%</div> <div>11%</div> </div>

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	Y3D	A	501	X	-	-	-
2	Y3D	B	501	X	-	-	-
2	Y3D	C	501	X	-	-	-

## 2 Entry composition [i](#)

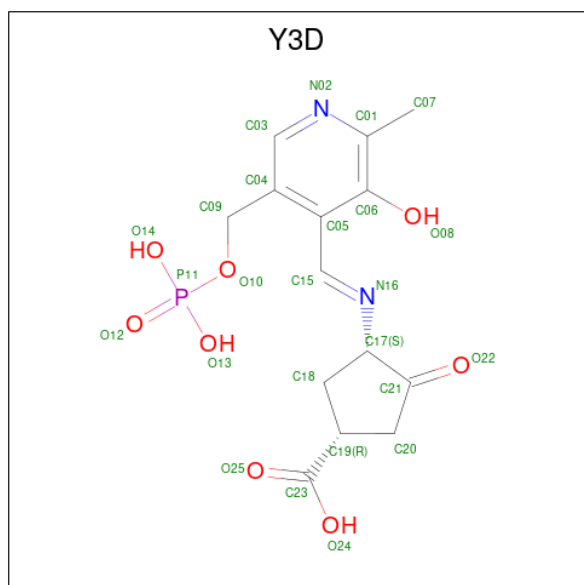
There are 3 unique types of molecules in this entry. The entry contains 10113 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	402	Total	C	N	O	S	0	3	0
			3160	2032	533	582	13			
1	B	402	Total	C	N	O	S	0	0	0
			3143	2020	530	581	12			
1	C	403	Total	C	N	O	S	0	1	0
			3153	2027	533	581	12			

- Molecule 2 is (1R,3S)-3-[(E)-({3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl} methylidene)amino]-4-oxocyclopentane-1-carboxylic acid (three-letter code: Y3D) (formula: C<sub>14</sub>H<sub>17</sub>N<sub>2</sub>O<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	14	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			25	14	2	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			25	14	2	8	1		

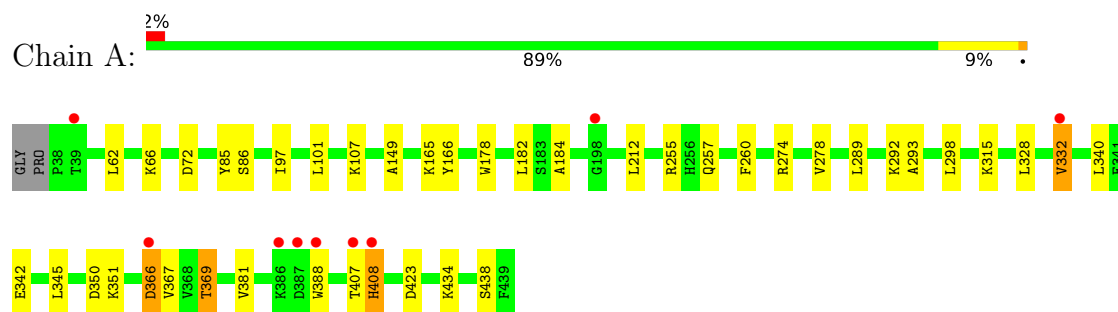
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	239	Total	O	0	0
			239	239		
3	B	161	Total	O	0	0
			161	161		
3	C	182	Total	O	0	0
			182	182		

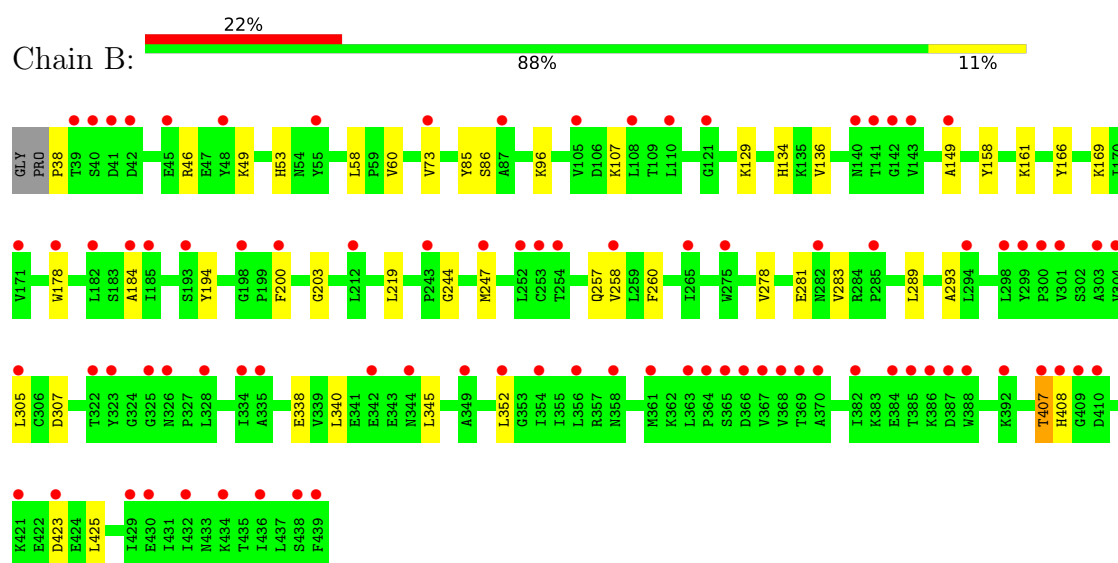
### 3 Residue-property plots [i](#)

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.

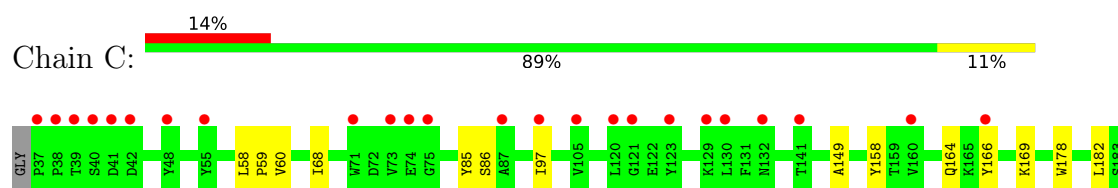
- Molecule 1: Ornithine aminotransferase, mitochondrial

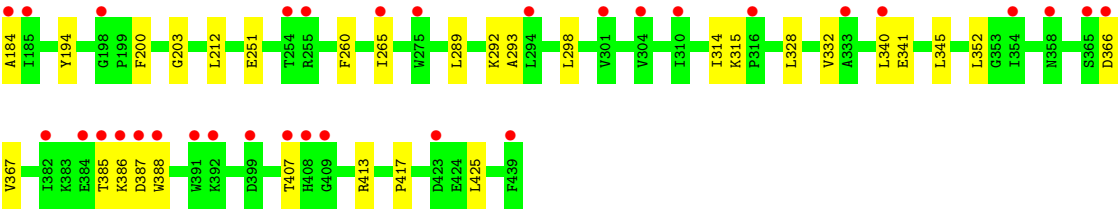


- Molecule 1: Ornithine aminotransferase, mitochondrial



- Molecule 1: Ornithine aminotransferase, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.71Å 192.71Å 56.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.18 – 1.96 48.18 – 1.96	Depositor EDS
% Data completeness (in resolution range)	90.8 (48.18-1.96) 91.3 (48.18-1.96)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.247 , 0.268 0.246 , 0.265	Depositor DCC
$R_{free}$ test set	3878 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 78.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1856e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: Y3D

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	0.32	0/3239	0.52	0/4398
1	B	0.27	0/3216	0.46	0/4366
1	C	0.28	0/3229	0.47	0/4384
All	All	0.29	0/9684	0.48	0/13148

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	3160	0	3173	24	0
1	B	3143	0	3148	26	0
1	C	3153	0	3162	23	0
2	A	25	0	0	1	0
2	B	25	0	0	1	0
2	C	25	0	0	1	0
3	A	239	0	0	7	0
3	B	161	0	0	5	0
3	C	182	0	0	7	0
All	All	10113	0	9483	76	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (76) 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:408:HIS:N	3:A:601:HOH:O	2.06	0.88
1:C:251:GLU:OE2	3:C:601:HOH:O	1.97	0.82
1:A:257:GLN:NE2	3:A:602:HOH:O	2.13	0.80
1:C:341:GLU:OE2	3:C:603:HOH:O	2.06	0.74
1:C:340:LEU:HD23	1:C:345:LEU:HD12	1.70	0.73
1:B:49:LYS:NZ	3:B:601:HOH:O	2.13	0.68
1:C:314:ILE:O	3:C:604:HOH:O	2.15	0.65
1:C:149:ALA:HB2	1:C:289:LEU:HD21	1.79	0.64
1:A:434:LYS:O	1:A:438:SER:OG	2.14	0.62
1:A:274:ARG:NH2	1:A:350:ASP:OD2	2.34	0.61
1:A:315:LYS:NZ	3:A:610:HOH:O	2.36	0.59
1:C:265:ILE:HG22	1:C:292:LYS:HD2	1.84	0.59
1:B:129:LYS:O	3:B:602:HOH:O	2.17	0.58
2:B:501:Y3D:O08	2:B:501:Y3D:N16	2.37	0.58
1:A:340:LEU:HD23	1:A:345:LEU:HD12	1.86	0.56
1:B:278:VAL:HG13	1:B:283:VAL:HB	1.88	0.56
1:A:149:ALA:HB2	1:A:289:LEU:HD21	1.87	0.56
1:A:328:LEU:O	1:A:332:VAL:HG13	2.07	0.54
1:A:178:TRP:CZ2	1:A:184:ALA:HA	2.43	0.53
2:C:501:Y3D:O08	2:C:501:Y3D:N16	2.41	0.53
1:C:169:LYS:HD3	1:C:203:GLY:HA2	1.91	0.53
2:A:501:Y3D:N16	2:A:501:Y3D:O08	2.40	0.52
1:B:149:ALA:HB2	1:B:289:LEU:HD21	1.92	0.52
1:B:161:LYS:HE3	1:B:257:GLN:HG3	1.91	0.51
1:B:178:TRP:CZ2	1:B:184:ALA:HA	2.46	0.51
1:C:85:TYR:O	1:C:292:LYS:HD3	2.09	0.51
1:B:244:GLY:HA2	1:B:247:MET:HE2	1.94	0.50
1:C:164:GLN:HB2	3:C:695:HOH:O	2.10	0.50
1:A:369:THR:N	1:A:381:VAL:O	2.42	0.49
1:C:328:LEU:O	1:C:332:VAL:HG13	2.12	0.49
1:B:86:SER:O	1:B:293:ALA:HB2	2.13	0.48
1:C:178:TRP:CZ2	1:C:184:ALA:HA	2.48	0.48
1:A:351:LYS:HG3	3:A:739:HOH:O	2.13	0.48
1:B:219:LEU:HD22	1:B:258:VAL:HG21	1.95	0.48
1:B:352:LEU:HB3	1:B:425:LEU:HD22	1.96	0.48
1:B:136:VAL:HB	1:B:305:LEU:HD23	1.96	0.47
1:A:107:LYS:HE2	3:A:663:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LYS:NZ	1:B:338:GLU:OE1	2.32	0.47
1:B:46:ARG:HD3	3:B:661:HOH:O	2.13	0.47
1:B:107:LYS:HE2	3:B:649:HOH:O	2.14	0.46
1:B:169:LYS:HD3	1:B:203:GLY:HA2	1.96	0.46
1:A:85:TYR:O	1:A:292:LYS:HD3	2.16	0.46
1:A:255:ARG:NE	3:A:617:HOH:O	2.48	0.46
1:A:423:ASP:OD1	1:A:423:ASP:N	2.47	0.46
1:A:165:LYS:HA	1:A:166:TYR:HA	1.63	0.46
1:A:367:VAL:HG13	1:A:388:TRP:CH2	2.51	0.46
1:B:407:THR:O	1:B:408:HIS:ND1	2.48	0.46
1:A:366:ASP:N	1:A:366:ASP:OD1	2.50	0.45
1:C:386:LYS:HA	3:C:622:HOH:O	2.15	0.45
1:C:97:ILE:HG22	1:C:298:LEU:HD22	1.98	0.45
1:C:158:TYR:OH	1:C:166:TYR:HA	2.17	0.44
1:B:38:PRO:O	1:B:73:VAL:HG21	2.17	0.44
1:B:53:HIS:HD2	3:B:749:HOH:O	1.99	0.44
1:B:247:MET:HG3	1:B:281:GLU:OE2	2.18	0.43
1:C:367:VAL:HB	1:C:388:TRP:CH2	2.53	0.43
1:C:413:ARG:NH2	3:C:614:HOH:O	2.42	0.43
1:C:86:SER:O	1:C:293:ALA:HB2	2.19	0.42
1:A:86:SER:O	1:A:293:ALA:HB2	2.19	0.42
1:C:352:LEU:HB3	1:C:425:LEU:HD22	2.01	0.42
1:A:62:LEU:HA	1:A:72:ASP:HA	2.01	0.42
1:A:66:LYS:HD3	1:A:66:LYS:HA	1.88	0.42
1:C:59:PRO:HG2	3:C:749:HOH:O	2.18	0.42
1:C:68:ILE:HA	1:C:417:PRO:HG2	2.01	0.42
1:B:340:LEU:HD23	1:B:345:LEU:HD12	2.01	0.41
1:A:342:GLU:HG3	3:A:604:HOH:O	2.19	0.41
1:C:58:LEU:O	1:C:60:VAL:N	2.52	0.41
1:B:134:HIS:HB2	1:B:307:ASP:HA	2.00	0.41
1:B:158:TYR:OH	1:B:166:TYR:HA	2.20	0.41
1:A:97:ILE:HG22	1:A:298:LEU:HD22	2.02	0.41
1:A:101:LEU:HD12	1:A:328:LEU:HD11	2.03	0.41
1:C:194:TYR:HB2	1:C:200:PHE:CE1	2.56	0.41
1:B:58:LEU:O	1:B:60:VAL:N	2.54	0.40
1:B:194:TYR:HB2	1:B:200:PHE:CE1	2.56	0.40
1:B:85:TYR:O	1:B:86:SER:HB2	2.21	0.40
1:C:385:THR:C	1:C:387:ASP:H	2.25	0.40
1:B:423:ASP:OD1	1:B:423:ASP:N	2.53	0.40

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	403/404 (100%)	379 (94%)	23 (6%)	1 (0%)	47	38
1	B	400/404 (99%)	378 (94%)	22 (6%)	0	100	100
1	C	402/404 (100%)	385 (96%)	17 (4%)	0	100	100
All	All	1205/1212 (99%)	1142 (95%)	62 (5%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	HIS

### 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	337/337 (100%)	328 (97%)	9 (3%)	44	34
1	B	334/337 (99%)	332 (99%)	2 (1%)	86	85
1	C	335/337 (99%)	329 (98%)	6 (2%)	59	53
All	All	1006/1011 (100%)	989 (98%)	17 (2%)	62	55

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	LEU
1	A	212[A]	LEU

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Mol	Chain	Res	Type
1	A	212[B]	LEU
1	A	260	PHE
1	A	278	VAL
1	A	332	VAL
1	A	366	ASP
1	A	369	THR
1	A	407	THR
1	B	260	PHE
1	B	407	THR
1	C	182	LEU
1	C	212	LEU
1	C	260	PHE
1	C	315	LYS
1	C	366	ASP
1	C	407	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	GLN
1	B	53	HIS
1	B	56	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

3 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	Y3D	C	501	-	21,26,26	4.58	8 (38%)	26,38,38	1.65	4 (15%)
2	Y3D	B	501	-	21,26,26	4.51	6 (28%)	26,38,38	1.79	4 (15%)
2	Y3D	A	501	-	21,26,26	4.49	5 (23%)	26,38,38	1.67	5 (19%)

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	Y3D	C	501	-	1/1/5/6	1/11/27/27	0/2/2/2
2	Y3D	B	501	-	1/1/5/6	3/11/27/27	0/2/2/2
2	Y3D	A	501	-	1/1/5/6	2/11/27/27	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	Y3D	C17-N16	-15.29	1.26	1.46
2	A	501	Y3D	C17-N16	-15.27	1.26	1.46
2	C	501	Y3D	C17-N16	-15.20	1.26	1.46
2	B	501	Y3D	C15-N16	10.07	1.46	1.27
2	A	501	Y3D	C15-N16	10.04	1.46	1.27
2	C	501	Y3D	C15-N16	9.99	1.46	1.27
2	B	501	Y3D	C05-C15	-7.36	1.32	1.46
2	C	501	Y3D	C05-C15	-7.23	1.32	1.46
2	A	501	Y3D	C05-C15	-7.19	1.33	1.46
2	C	501	Y3D	P11-O12	4.45	1.64	1.50
2	A	501	Y3D	C05-C04	-2.64	1.38	1.42
2	B	501	Y3D	P11-O13	2.54	1.64	1.54
2	C	501	Y3D	C05-C04	-2.51	1.38	1.42
2	B	501	Y3D	C05-C04	-2.33	1.39	1.42
2	B	501	Y3D	C20-C21	2.25	1.54	1.51
2	C	501	Y3D	P11-O14	-2.22	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	Y3D	P11-O13	2.18	1.63	1.54
2	C	501	Y3D	P11-O13	-2.16	1.46	1.54
2	C	501	Y3D	C20-C21	2.08	1.54	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	Y3D	C20-C19-C23	4.67	124.62	115.17
2	C	501	Y3D	C20-C19-C23	4.51	124.30	115.17
2	A	501	Y3D	C20-C19-C23	4.24	123.74	115.17
2	B	501	Y3D	C05-C06-C01	-3.57	117.98	120.19
2	C	501	Y3D	C05-C06-C01	-3.47	118.04	120.19
2	A	501	Y3D	C17-N16-C15	3.40	122.22	117.31
2	A	501	Y3D	C05-C06-C01	-3.20	118.20	120.19
2	B	501	Y3D	C17-N16-C15	3.14	121.83	117.31
2	C	501	Y3D	C17-N16-C15	2.93	121.54	117.31
2	B	501	Y3D	C04-C03-N02	-2.76	119.22	123.82
2	C	501	Y3D	C04-C03-N02	-2.66	119.38	123.82
2	A	501	Y3D	C05-C15-N16	-2.27	117.96	123.01
2	A	501	Y3D	C04-C03-N02	-2.22	120.12	123.82

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	Y3D	C17
2	B	501	Y3D	C17
2	C	501	Y3D	C17

All (6) torsion outliers are listed below:

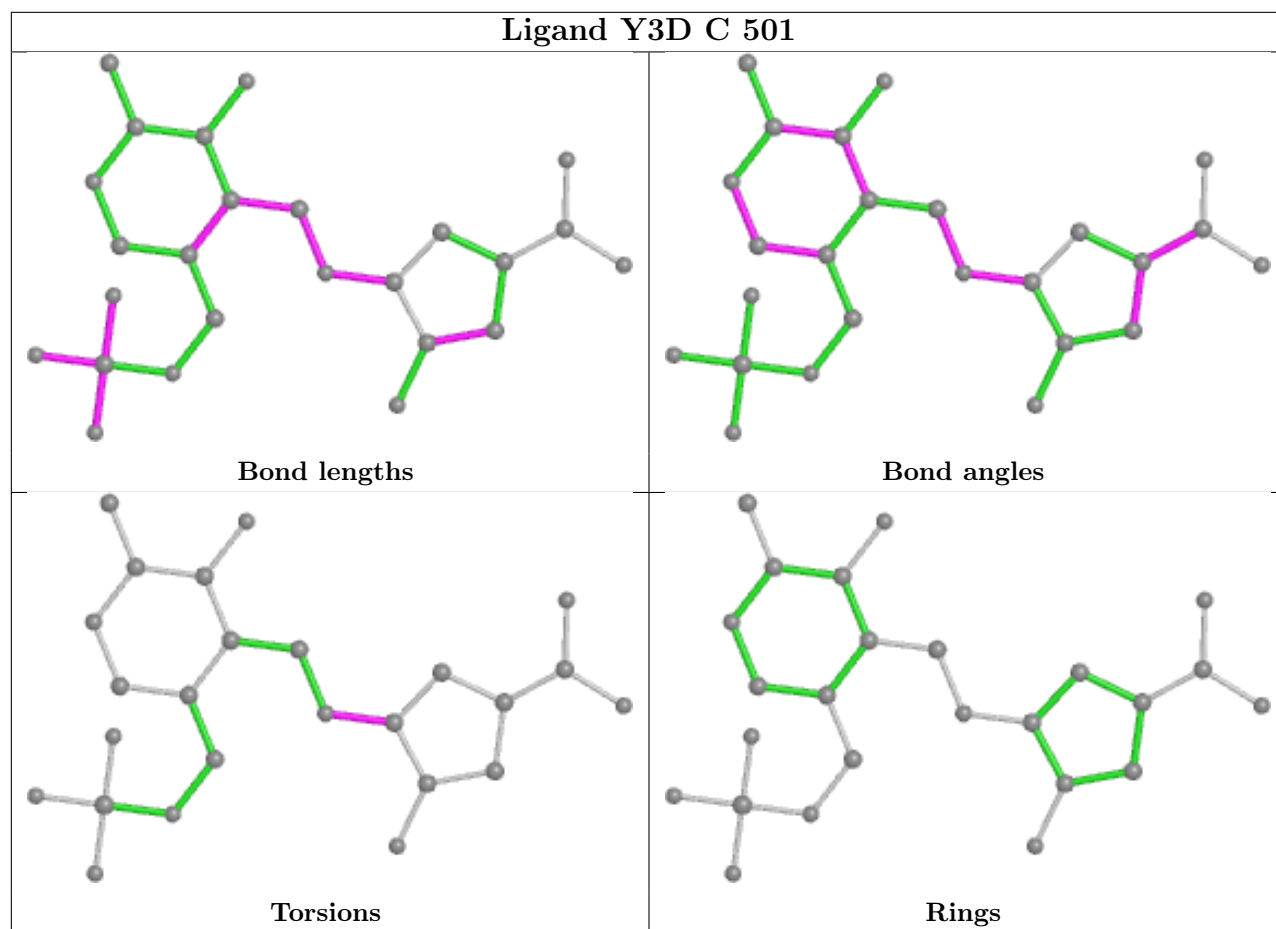
Mol	Chain	Res	Type	Atoms
2	A	501	Y3D	C18-C17-N16-C15
2	B	501	Y3D	C18-C17-N16-C15
2	C	501	Y3D	C18-C17-N16-C15
2	B	501	Y3D	C09-O10-P11-O12
2	A	501	Y3D	C21-C17-N16-C15
2	B	501	Y3D	C21-C17-N16-C15

There are no ring outliers.

3 monomers are involved in 3 short contacts:

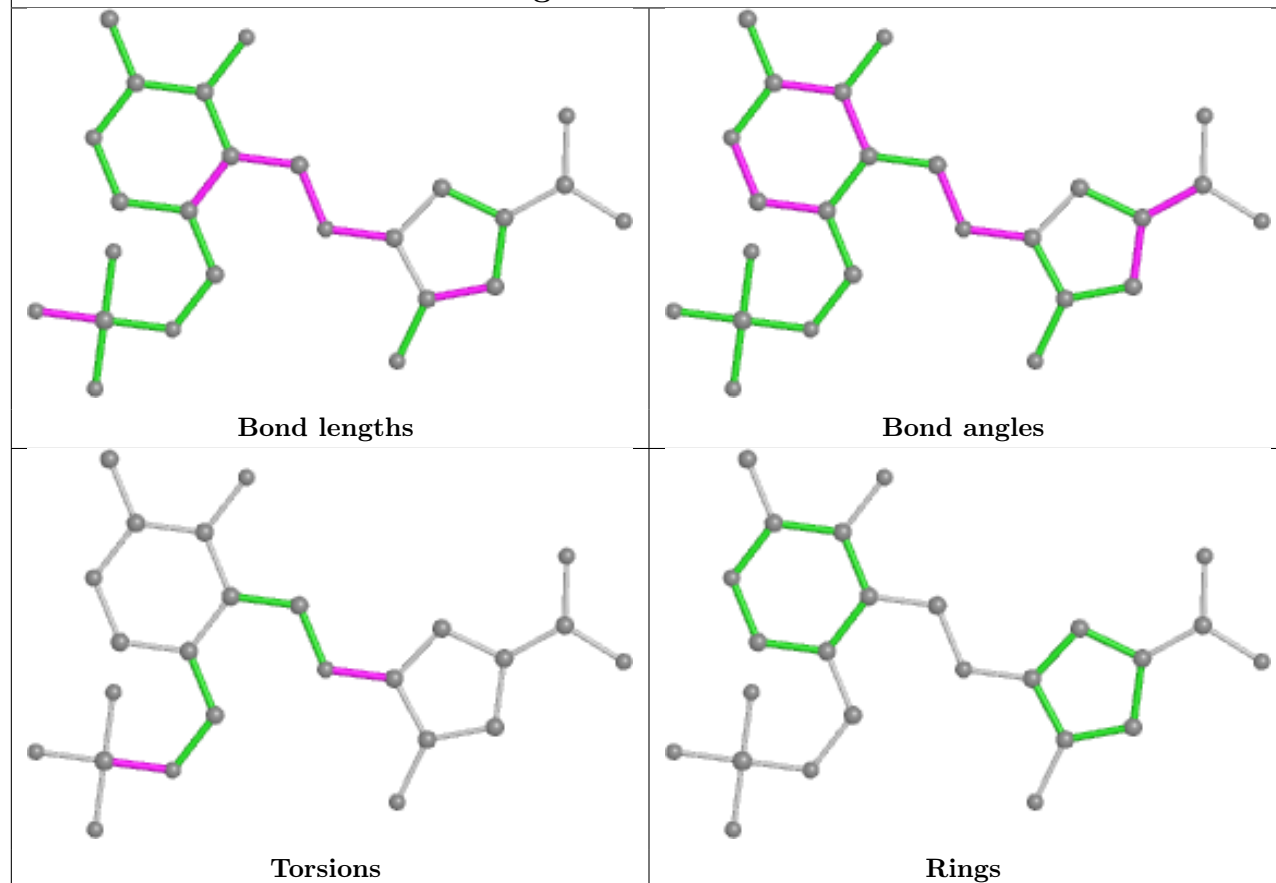
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	Y3D	1	0
2	B	501	Y3D	1	0
2	A	501	Y3D	1	0

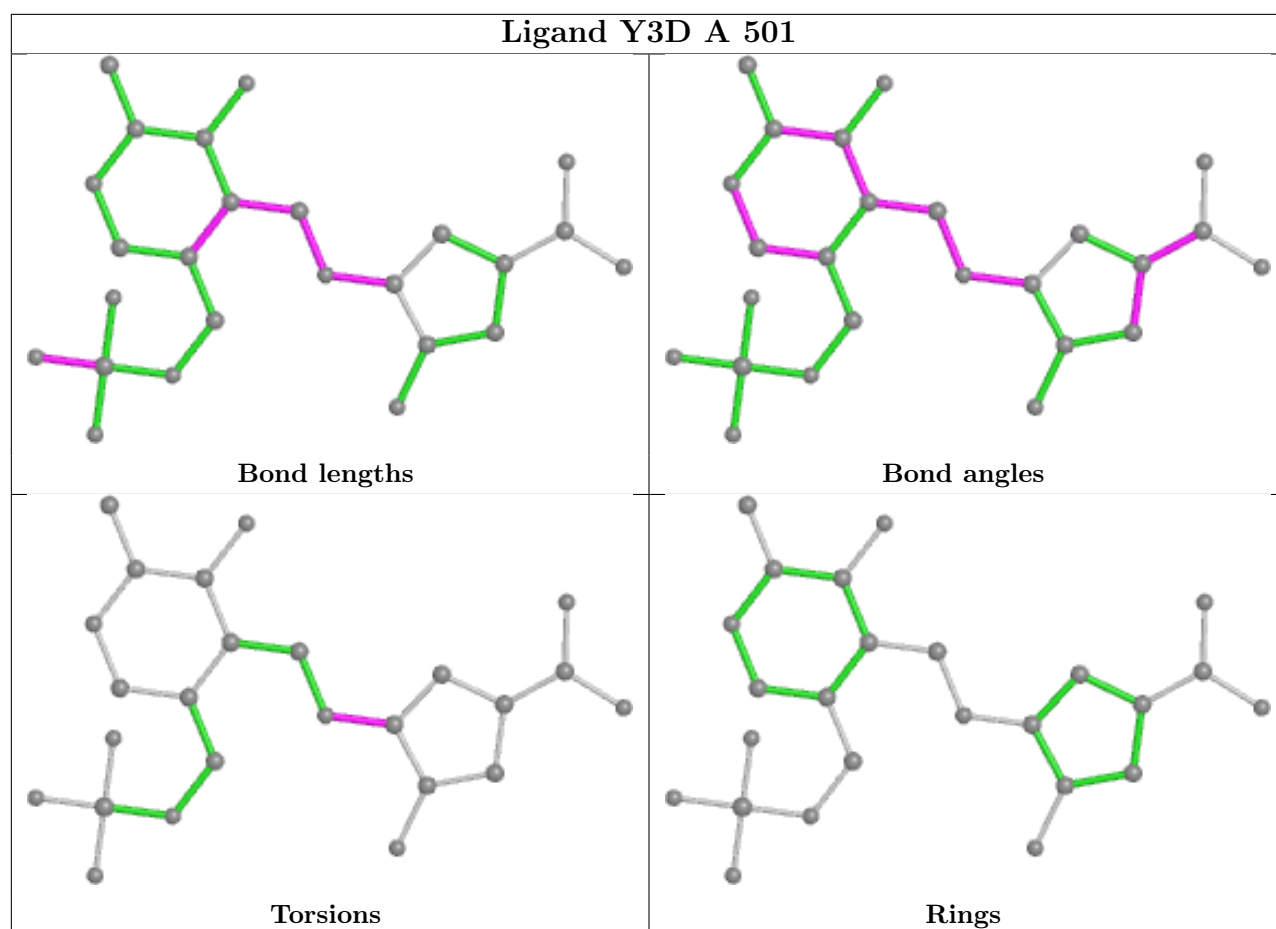
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 Y3D 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, 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	402/404 (99%)	-0.03	9 (2%) 62 70	8, 20, 39, 62	0
1	B	402/404 (99%)	1.30	88 (21%) 0 0	33, 43, 62, 80	0
1	C	403/404 (99%)	1.03	56 (13%) 2 4	29, 41, 60, 83	0
All	All	1207/1212 (99%)	0.77	153 (12%) 3 6	8, 39, 58, 83	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	PRO	9.2
1	A	387	ASP	7.6
1	B	388	TRP	6.4
1	B	387	ASP	6.3
1	C	387	ASP	6.2
1	B	365	SER	6.0
1	C	198	GLY	5.7
1	C	408	HIS	5.5
1	B	385	THR	5.3
1	C	73	VAL	5.3
1	B	141	THR	5.0
1	C	40	SER	4.9
1	B	407	THR	4.9
1	B	301	VAL	4.8
1	B	41	ASP	4.7
1	B	265	ILE	4.6
1	B	436	ILE	4.6
1	B	198	GLY	4.5
1	B	87	ALA	4.3
1	C	388	TRP	4.3
1	C	41	ASP	4.3
1	C	48	TYR	4.2
1	B	354	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	392	LYS	4.0
1	C	38	PRO	4.0
1	B	423	ASP	3.9
1	B	367	VAL	3.9
1	C	132	ASN	3.7
1	C	382	ILE	3.7
1	B	48	TYR	3.7
1	B	185	ILE	3.6
1	B	298	LEU	3.6
1	C	386	LYS	3.6
1	C	439	PHE	3.5
1	C	275	TRP	3.5
1	C	354	ILE	3.4
1	C	333	ALA	3.4
1	B	366	ASP	3.4
1	B	386	LYS	3.4
1	C	39	THR	3.4
1	B	299	TYR	3.4
1	B	408	HIS	3.4
1	B	143	VAL	3.4
1	B	323	TYR	3.3
1	B	358	ASN	3.3
1	C	71	TRP	3.3
1	B	432	ILE	3.3
1	B	328	LEU	3.3
1	A	198	GLY	3.3
1	B	73	VAL	3.2
1	C	75	GLY	3.2
1	B	430	GLU	3.2
1	C	385	THR	3.2
1	B	40	SER	3.2
1	C	399	ASP	3.2
1	B	363	LEU	3.1
1	C	340	LEU	3.1
1	B	322	THR	3.1
1	B	110	LEU	3.1
1	C	87	ALA	3.1
1	C	423	ASP	3.1
1	B	342	GLU	3.1
1	B	275	TRP	3.1
1	C	391	TRP	3.1
1	C	301	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	370	ALA	3.1
1	C	55	TYR	3.0
1	B	361	MET	3.0
1	B	300	PRO	3.0
1	C	141	THR	2.9
1	B	140	ASN	2.9
1	B	45	GLU	2.9
1	A	408	HIS	2.8
1	B	304	VAL	2.8
1	C	160	VAL	2.8
1	A	386	LYS	2.8
1	C	366	ASP	2.8
1	B	439	PHE	2.8
1	B	344	ASN	2.8
1	A	366	ASP	2.7
1	C	254	THR	2.7
1	C	121	GLY	2.7
1	B	178	TRP	2.7
1	B	409	GLY	2.6
1	A	388	TRP	2.6
1	B	294	LEU	2.6
1	C	294	LEU	2.6
1	A	39	THR	2.5
1	B	184	ALA	2.5
1	B	352	LEU	2.5
1	B	282	ASN	2.5
1	B	171	VAL	2.5
1	C	123	TYR	2.5
1	B	149	ALA	2.5
1	B	335	ALA	2.5
1	B	39	THR	2.5
1	B	182	LEU	2.5
1	B	349	ALA	2.4
1	B	382	ILE	2.4
1	B	305	LEU	2.4
1	B	384	GLU	2.4
1	B	42	ASP	2.4
1	B	55	TYR	2.4
1	B	438	SER	2.4
1	B	429	ILE	2.4
1	B	392	LYS	2.4
1	C	384	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	310	ILE	2.4
1	C	105	VAL	2.3
1	C	184	ALA	2.3
1	B	105	VAL	2.3
1	B	252	LEU	2.3
1	C	316	PRO	2.3
1	B	325	GLY	2.3
1	B	193	SER	2.3
1	B	434	LYS	2.3
1	C	42	ASP	2.3
1	C	409	GLY	2.3
1	A	407	THR	2.3
1	B	243	PRO	2.3
1	C	407	THR	2.3
1	B	356	LEU	2.3
1	B	334	ILE	2.2
1	B	212	LEU	2.2
1	C	358	ASN	2.2
1	B	369	THR	2.2
1	B	247	MET	2.2
1	B	421	LYS	2.2
1	A	332	VAL	2.2
1	C	265	ILE	2.2
1	B	142	GLY	2.2
1	C	166	TYR	2.2
1	B	364	PRO	2.1
1	B	108	LEU	2.1
1	B	200	PHE	2.1
1	C	365	SER	2.1
1	B	410	ASP	2.1
1	C	120	LEU	2.1
1	B	121	GLY	2.1
1	B	254	THR	2.1
1	B	368	VAL	2.1
1	B	303	ALA	2.1
1	B	253	CYS	2.1
1	C	255	ARG	2.0
1	B	326	ASN	2.0
1	B	258	VAL	2.0
1	C	304	VAL	2.0
1	B	285	PRO	2.0
1	C	129	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	130	LEU	2.0
1	C	97	ILE	2.0
1	C	185	ILE	2.0
1	C	74	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

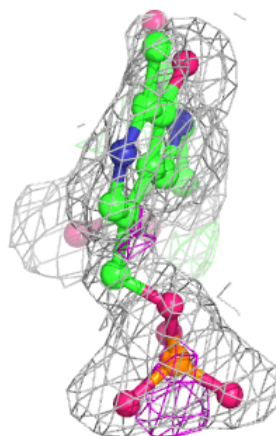
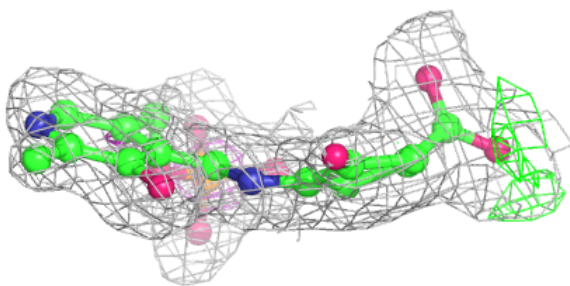
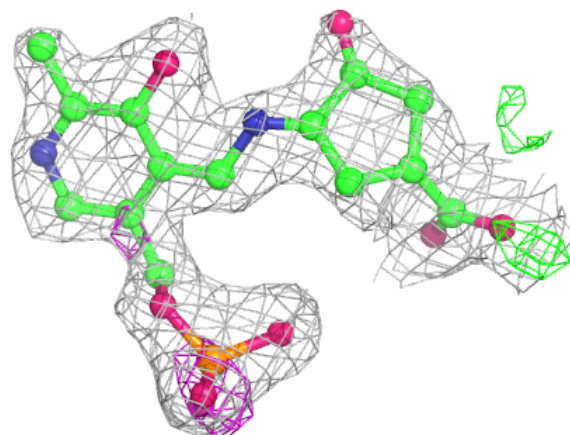
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	Y3D	C	501	25/25	0.92	0.13	22,30,47,50	0
2	Y3D	B	501	25/25	0.93	0.13	19,29,44,49	0
2	Y3D	A	501	25/25	0.95	0.15	8,20,38,41	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 Y3D C 501:**

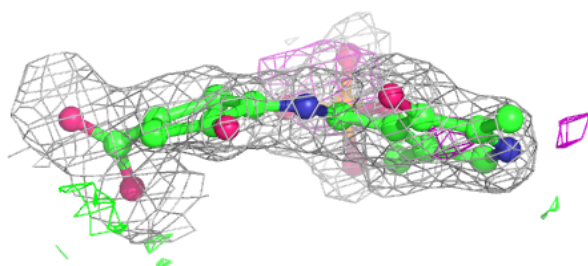
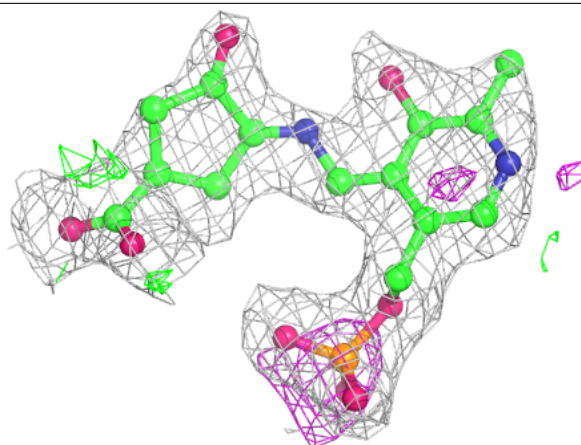
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





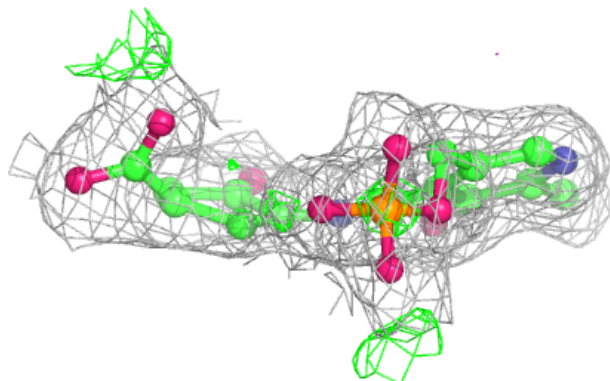
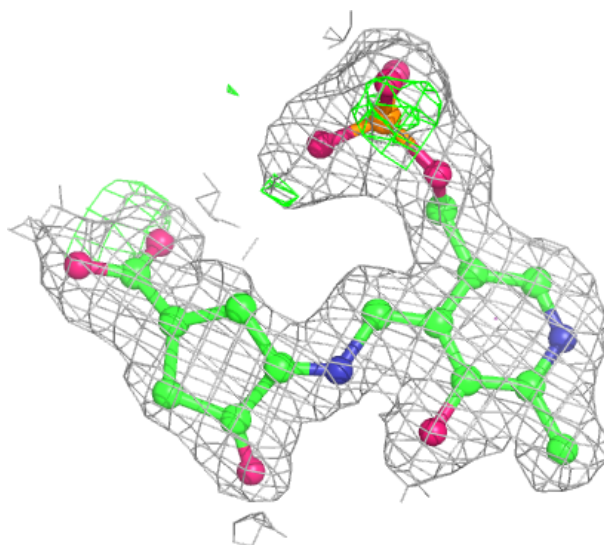
**Electron density around Y3D B 501:**

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



**Electron density around Y3D A 501:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.