



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2022 – 06:09 PM EDT

PDB ID : 7TDL  
Title : M379A mutant tyrosine phenol-lyase complexed with 3-bromo-DL-phenylalane  
Authors : Phillips, R.S.  
Deposited on : 2022-01-01  
Resolution : 1.60 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 : 2.28.1  
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) : 2.28.1

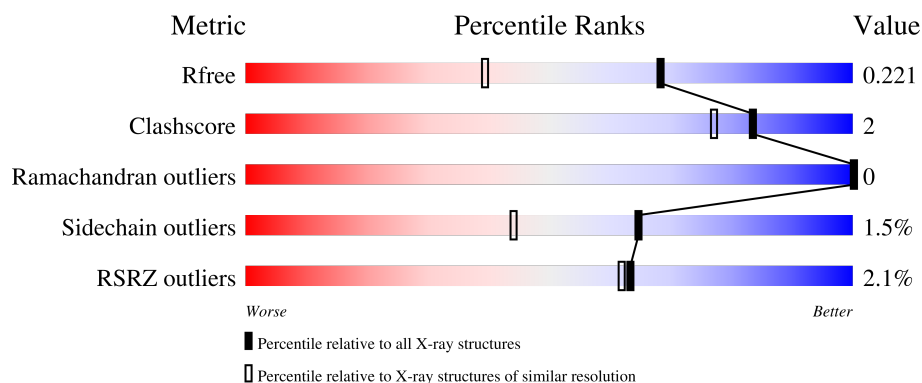
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	456	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	B	456	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
1	C	456	<div> <div></div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	D	456	<div> <div>%</div> <div> <div></div> <div>96%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 31090 atoms, of which 14679 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 Tyrosine phenol-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	456	Total	C	H	N	O	S	0	10	0
			7289	2321	3628	633	680	27			
1	B	456	Total	C	H	N	O	S	0	12	0
			7306	2323	3636	639	681	27			
1	C	456	Total	C	H	N	O	S	0	15	0
			7358	2340	3667	640	684	27			
1	D	456	Total	C	H	N	O	S	0	14	0
			7321	2330	3640	638	684	29			

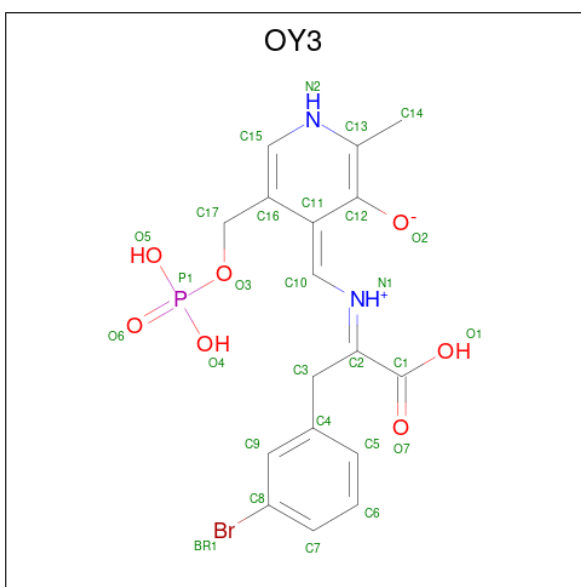
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ALA	GLU	conflict	UNP P31013
A	379	ALA	MET	engineered mutation	UNP P31013
B	205	ALA	GLU	conflict	UNP P31013
B	379	ALA	MET	engineered mutation	UNP P31013
C	205	ALA	GLU	conflict	UNP P31013
C	379	ALA	MET	engineered mutation	UNP P31013
D	205	ALA	GLU	conflict	UNP P31013
D	379	ALA	MET	engineered mutation	UNP P31013

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

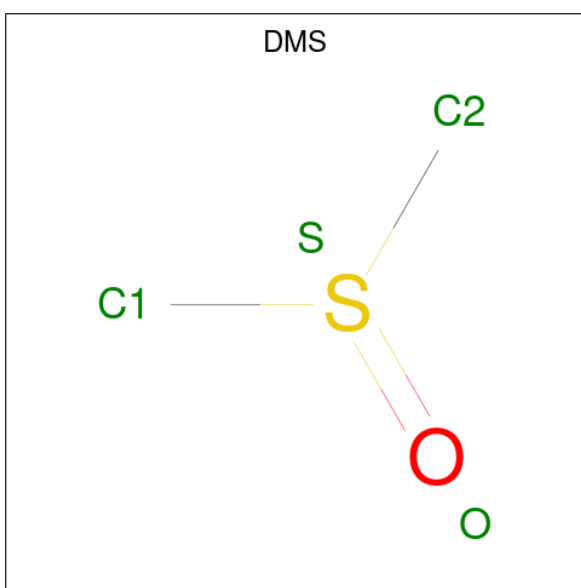
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	K	0	0
			2	2		
2	C	2	Total	K	0	0
			2	2		

- Molecule 3 is (4Z)-4-({[(1E)-2-(3-bromophenyl)-1-carboxyethylidene]azaniumyl}methylidene)-2-methyl-5-[(phosphonooxy)methyl]-1,4-dihydropyridin-3-olate (three-letter code: OY3) (formula: C<sub>17</sub>H<sub>18</sub>BrN<sub>2</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Br	C	H	N	O	P		
3	A	1	86	2	34	30	4	14	2	0	1
3	B	1	86	2	34	30	4	14	2	0	1

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
4	A	1	10	2	6	1	1	0	0
4	C	1	10	2	6	1	1	0	0

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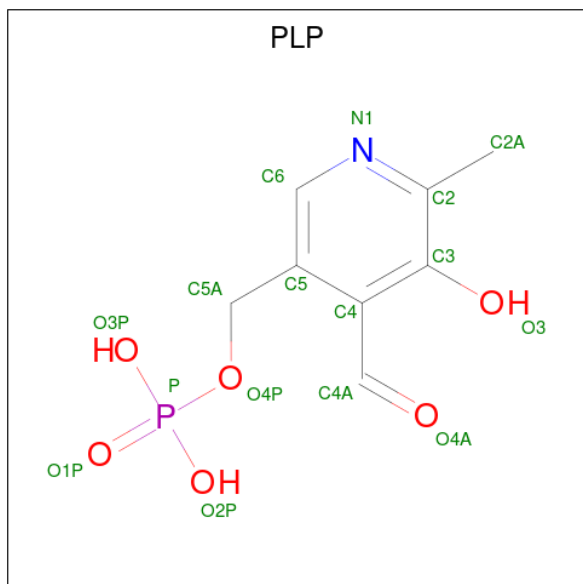
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
4	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	P	0	1
			23	8	8	1	5	1		
6	C	1	Total	C	H	N	O	P	0	0
			23	8	8	1	5	1		
6	D	1	Total	C	H	N	O	P	0	0
			23	8	8	1	5	1		

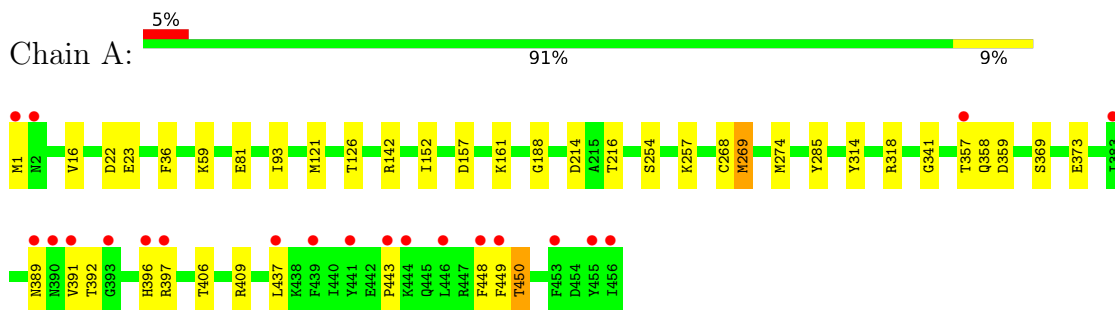
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	341	Total 341	O 341	0	27
7	B	286	Total 286	O 286	0	10
7	C	465	Total 465	O 465	0	29
7	D	436	Total 436	O 436	0	25

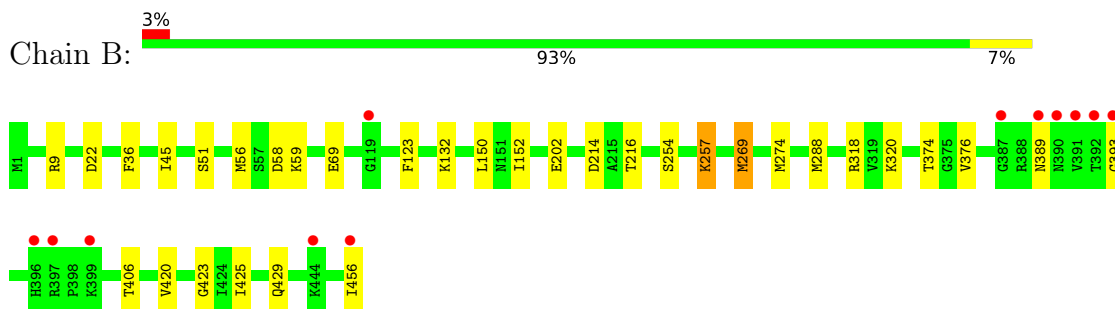
### 3 Residue-property plots [i](#)

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.

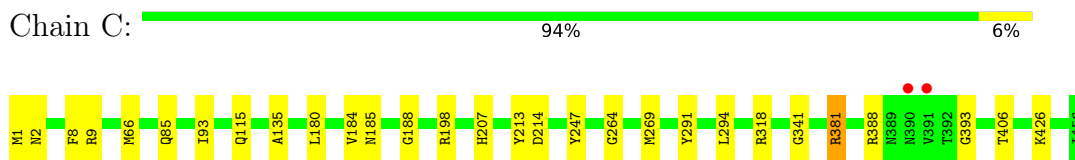
- Molecule 1: Tyrosine phenol-lyase



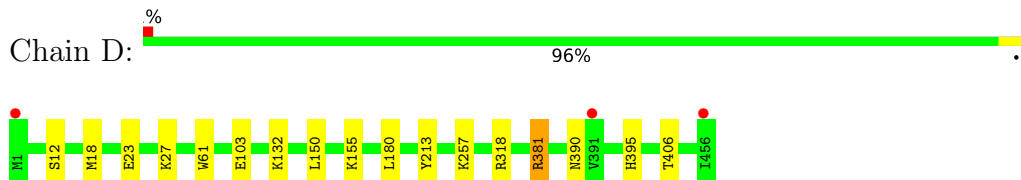
- Molecule 1: Tyrosine phenol-lyase



- Molecule 1: Tyrosine phenol-lyase



- Molecule 1: Tyrosine phenol-lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.25Å 82.87Å 94.33Å 113.16° 96.54° 102.21°	Depositor
Resolution (Å)	58.41 – 1.60 58.41 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (58.41-1.60) 98.6 (58.41-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.177 , 0.221 0.178 , 0.221	Depositor DCC
$R_{free}$ test set	1985 reflections (0.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	31090	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, CL, PLP, OY3, DMS

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	0.69	1/3767 (0.0%)	0.75	0/5073
1	B	0.61	1/3776 (0.0%)	0.71	1/5081 (0.0%)
1	C	0.75	1/3809 (0.0%)	0.79	0/5126
1	D	0.74	0/3793	0.78	0/5104
All	All	0.70	3/15145 (0.0%)	0.76	1/20384 (0.0%)

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	C	0	1
1	D	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	CYS	CB-SG	-6.96	1.70	1.82
1	B	69	GLU	CB-CG	6.52	1.64	1.52
1	C	291	TYR	CE1-CZ	5.56	1.45	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ASP	CB-CG-OD1	6.96	124.56	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	381	ARG	Sidechain
1	D	381	ARG	Sidechain
1	D	395	HIS	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3661	3628	3630	32	0
1	B	3670	3636	3634	20	0
1	C	3691	3667	3659	17	0
1	D	3681	3640	3634	9	0
2	A	2	0	0	0	0
2	C	2	0	0	0	0
3	A	56	30	0	6	0
3	B	56	30	0	1	0
4	A	4	6	6	0	0
4	C	8	12	12	0	0
4	D	4	6	6	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	B	15	8	7	1	0
6	C	15	8	7	1	0
6	D	15	8	7	2	0
7	A	341	0	0	6	0
7	B	286	0	0	2	0
7	C	465	0	0	7	0
7	D	436	0	0	1	0
All	All	16411	14679	14602	72	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (72) 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:391:VAL:HG13	1:A:392:THR:HG23	1.66	0.77
1:A:214:ASP:OD1	1:A:216[B]:THR:HG23	1.88	0.74
1:B:123:PHE:HB2	6:B:502[A]:PLP:H2A3	1.82	0.61
1:C:184:VAL:HG13	7:C:840:HOH:O	2.04	0.57
1:A:16[A]:VAL:HG11	1:C:9:ARG:HG3	1.86	0.56
1:A:389:ASN:OD1	1:A:391:VAL:HG12	2.05	0.56
1:A:443:PRO:HG2	1:A:450:THR:HG23	1.89	0.55
1:C:1:MET:HE2	7:C:952:HOH:O	2.07	0.55
1:B:214:ASP:OD1	1:B:216[B]:THR:HG23	2.06	0.54
1:A:257:LYS:HZ1	3:A:501[B]:OY3:C10	2.21	0.53
1:B:45:ILE:HB	1:B:376:VAL:HG22	1.89	0.53
1:A:443:PRO:CG	1:A:450:THR:HG23	2.38	0.53
1:B:59:LYS:HD3	1:C:66[B]:MET:SD	2.50	0.52
1:B:257[B]:LYS:HZ1	3:B:501[B]:OY3:C10	2.22	0.52
1:D:257:LYS:NZ	6:D:502:PLP:O3	2.42	0.52
1:A:257:LYS:NZ	3:A:501[B]:OY3:C10	2.75	0.50
1:B:269:MET:HE2	1:B:274:MET:HG2	1.94	0.49
1:A:16[A]:VAL:HG22	1:C:8:PHE:HA	1.95	0.49
1:A:448:PHE:CE2	3:A:501[A]:OY3:BR1	3.20	0.49
1:D:23:GLU:O	1:D:27:LYS:HG2	2.13	0.49
1:A:369:SER:O	1:A:373:GLU:HG2	2.12	0.48
1:A:22:ASP:OD1	1:A:23:GLU:N	2.47	0.47
1:C:185:ASN:HB2	7:C:819:HOH:O	2.14	0.47
1:A:257:LYS:HZ1	3:A:501[A]:OY3:C10	2.28	0.47
1:B:389:ASN:O	1:B:393:GLY:N	2.45	0.47
1:A:188:GLY:O	1:A:341:GLY:HA3	2.16	0.46
1:A:357[B]:THR:HG22	1:A:358:GLN:N	2.30	0.46
1:C:2:ASN:ND2	7:C:607:HOH:O	2.47	0.46
1:C:188:GLY:O	1:C:341:GLY:HA3	2.15	0.46
1:D:61:TRP:CE2	4:D:501:DMS:H11	2.50	0.46
1:A:449:PHE:CD1	1:B:288:MET:SD	3.09	0.46
1:B:150:LEU:HG	1:B:152:ILE:HG23	1.98	0.45
1:C:207:HIS:HD2	7:C:878:HOH:O	1.99	0.45
1:D:180:LEU:O	1:D:213:TYR:HA	2.17	0.45
1:A:121:MET:O	7:A:601:HOH:O	2.20	0.44
1:A:142:ARG:HD2	1:A:157:ASP:HB2	2.00	0.44
1:A:257:LYS:NZ	3:A:501[A]:OY3:C10	2.81	0.43
1:A:274:MET:HE2	7:A:829:HOH:O	2.18	0.43
1:C:388:ARG:HD2	1:C:393:GLY:O	2.18	0.43
1:A:36:PHE:CE1	3:A:501[A]:OY3:BR1	3.27	0.43
1:D:18[A]:MET:HE3	7:D:779[A]:HOH:O	2.19	0.43
1:A:216[B]:THR:HG22	1:A:254:SER:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:HIS:HE1	7:A:867:HOH:O	2.02	0.42
1:B:216[A]:THR:HG23	1:B:254:SER:HB3	2.01	0.42
1:A:16[A]:VAL:HG12	7:A:785:HOH:O	2.19	0.42
1:A:285:TYR:OH	1:B:132:LYS:NZ	2.41	0.42
1:B:456:ILE:HD11	7:B:867:HOH:O	2.20	0.42
1:C:85:GLN:HG3	1:C:93[B]:ILE:CD1	2.50	0.42
1:D:103:GLU:OE2	6:D:502:PLP:H6	2.20	0.42
1:A:81:GLU:HA	1:A:93[A]:ILE:HG21	2.01	0.42
1:A:269:MET:HB2	1:A:274:MET:CE	2.50	0.42
1:B:22:ASP:HB2	7:B:856:HOH:O	2.19	0.42
1:C:264:GLY:HA2	1:C:294:LEU:HD21	2.01	0.41
1:A:161:LYS:HE3	7:A:739:HOH:O	2.19	0.41
1:C:180:LEU:O	1:C:213:TYR:HA	2.20	0.41
1:A:437:LEU:O	7:A:602:HOH:O	2.22	0.41
1:A:359:ASP:OD2	1:A:397:ARG:NH2	2.54	0.41
1:B:51:SER:HB2	1:B:257[B]:LYS:HE3	2.03	0.41
1:B:425:ILE:O	1:B:429:GLN:HG3	2.20	0.41
1:C:115:GLN:O	1:C:135:ALA:HA	2.20	0.41
1:B:376:VAL:HG21	1:B:420:VAL:HG22	2.03	0.41
1:A:59:LYS:HE2	7:C:960:HOH:O	2.21	0.41
1:B:56:MET:O	1:D:12:SER:HA	2.21	0.41
1:A:314:TYR:OH	1:A:409:ARG:HD3	2.21	0.41
1:B:45:ILE:O	1:B:376:VAL:HA	2.21	0.40
1:C:426:LYS:HG3	7:C:738:HOH:O	2.20	0.40
1:D:390[A]:ASN:OD1	1:D:390[A]:ASN:N	2.54	0.40
1:C:198[A]:ARG:HG2	1:C:247:TYR:CZ	2.56	0.40
1:C:214:ASP:OD2	6:C:502:PLP:N1	2.53	0.40
1:D:150:LEU:O	1:D:155:LYS:HE3	2.21	0.40
1:B:374:THR:CG2	1:B:423:GLY:HA3	2.51	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	464/456 (102%)	451 (97%)	13 (3%)	0	100	100
1	B	466/456 (102%)	454 (97%)	12 (3%)	0	100	100
1	C	469/456 (103%)	458 (98%)	11 (2%)	0	100	100
1	D	468/456 (103%)	457 (98%)	11 (2%)	0	100	100
All	All	1867/1824 (102%)	1820 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	387/377 (103%)	380 (98%)	7 (2%)	59	36
1	B	387/377 (103%)	378 (98%)	9 (2%)	50	25
1	C	391/377 (104%)	387 (99%)	4 (1%)	76	61
1	D	389/377 (103%)	385 (99%)	4 (1%)	76	61
All	All	1554/1508 (103%)	1530 (98%)	24 (2%)	65	44

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	126	THR
1	A	152	ILE
1	A	269	MET
1	A	318	ARG
1	A	406	THR
1	A	450	THR
1	B	9[A]	ARG
1	B	9[B]	ARG
1	B	36	PHE
1	B	202	GLU
1	B	257[A]	LYS
1	B	257[B]	LYS

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Mol	Chain	Res	Type
1	B	269	MET
1	B	318	ARG
1	B	406	THR
1	C	269	MET
1	C	318	ARG
1	C	381	ARG
1	C	406	THR
1	D	132	LYS
1	D	318	ARG
1	D	381	ARG
1	D	406	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 18 ligands modelled in this entry, 7 are monoatomic - leaving 11 for Mogul analysis.

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
6	PLP	B	502[A]	1	15,15,16	2.24	5 (33%)	20,22,23	1.31	2 (10%)
3	OY3	A	501[B]	-	25,29,29	2.39	3 (12%)	31,41,41	1.09	2 (6%)
4	DMS	C	503	-	3,3,3	0.42	0	3,3,3	0.80	0
4	DMS	C	504	-	3,3,3	0.75	0	3,3,3	0.85	0
4	DMS	D	501	-	3,3,3	0.41	0	3,3,3	1.69	1 (33%)
3	OY3	A	501[A]	-	25,29,29	2.59	3 (12%)	31,41,41	1.05	1 (3%)
6	PLP	C	502	1	15,15,16	2.01	4 (26%)	20,22,23	1.42	3 (15%)
4	DMS	A	504	-	3,3,3	0.80	0	3,3,3	1.08	0
3	OY3	B	501[B]	-	25,29,29	2.55	3 (12%)	31,41,41	0.99	1 (3%)
6	PLP	D	502	1	15,15,16	2.22	5 (33%)	20,22,23	1.16	1 (5%)
3	OY3	B	501[C]	-	25,29,29	2.52	3 (12%)	31,41,41	1.07	3 (9%)

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
6	PLP	B	502[A]	1	-	5/6/6/8	0/1/1/1
3	OY3	A	501[B]	-	-	0/11/19/19	0/2/2/2
6	PLP	C	502	1	-	0/6/6/8	0/1/1/1
3	OY3	A	501[A]	-	-	0/11/19/19	0/2/2/2
3	OY3	B	501[B]	-	-	0/11/19/19	0/2/2/2
6	PLP	D	502	1	-	0/6/6/8	0/1/1/1
3	OY3	B	501[C]	-	-	0/11/19/19	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501[A]	OY3	C1-C2	-10.82	1.35	1.52
3	B	501[B]	OY3	C1-C2	-10.64	1.36	1.52
3	B	501[C]	OY3	C1-C2	-10.63	1.36	1.52
3	A	501[B]	OY3	C1-C2	-10.12	1.36	1.52
3	A	501[A]	OY3	C12-C13	-5.11	1.36	1.40
3	B	501[B]	OY3	C12-C13	-4.99	1.36	1.40
6	B	502[A]	PLP	C4A-C4	4.93	1.61	1.51
6	C	502	PLP	C4A-C4	4.69	1.61	1.51
3	A	501[B]	OY3	C12-C13	-4.43	1.36	1.40
3	B	501[C]	OY3	C12-C13	-4.37	1.36	1.40
6	D	502	PLP	C4A-C4	4.08	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	502	PLP	C6-N1	3.61	1.42	1.34
6	D	502	PLP	C2A-C2	3.52	1.56	1.50
3	B	501[B]	OY3	O2-C12	-3.50	1.23	1.35
3	A	501[A]	OY3	O2-C12	-3.46	1.24	1.35
6	C	502	PLP	C6-N1	3.45	1.41	1.34
6	D	502	PLP	C5-C4	-3.44	1.36	1.40
6	B	502[A]	PLP	C2A-C2	3.40	1.56	1.50
3	B	501[C]	OY3	O2-C12	-3.28	1.24	1.35
3	A	501[B]	OY3	O2-C12	-3.14	1.25	1.35
6	B	502[A]	PLP	C6-N1	3.10	1.41	1.34
6	D	502	PLP	C5A-C5	2.96	1.58	1.50
6	C	502	PLP	O3-C3	2.55	1.42	1.37
6	B	502[A]	PLP	C5-C4	-2.43	1.37	1.40
6	B	502[A]	PLP	C5A-C5	2.34	1.57	1.50
6	C	502	PLP	C5A-C5	2.06	1.56	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	502	PLP	O4P-C5A-C5	3.46	115.95	109.35
3	A	501[A]	OY3	C3-C2-N1	-3.23	117.77	125.81
3	B	501[B]	OY3	C3-C2-N1	-3.05	118.22	125.81
6	B	502[A]	PLP	C4A-C4-C5	2.86	123.89	120.94
3	A	501[B]	OY3	C3-C2-N1	-2.72	119.04	125.81
3	B	501[C]	OY3	C3-C2-N1	-2.65	119.22	125.81
3	A	501[B]	OY3	C14-C13-C12	2.45	123.91	120.89
3	B	501[C]	OY3	C14-C13-C12	2.43	123.89	120.89
6	B	502[A]	PLP	C4A-C4-C3	-2.41	116.42	120.50
4	D	501	DMS	C2-S-C1	-2.37	86.24	98.44
6	C	502	PLP	C2A-C2-C3	-2.27	118.08	120.89
3	B	501[C]	OY3	O5-P1-O4	2.14	115.83	107.64
6	C	502	PLP	C6-N1-C2	-2.13	115.22	119.17
6	D	502	PLP	C4A-C4-C3	-2.04	117.03	120.50

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	502[A]	PLP	C4-C5-C5A-O4P
6	B	502[A]	PLP	C6-C5-C5A-O4P
6	B	502[A]	PLP	C5A-O4P-P-O2P
6	B	502[A]	PLP	C5A-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
6	B	502[A]	PLP	C5A-O4P-P-O1P

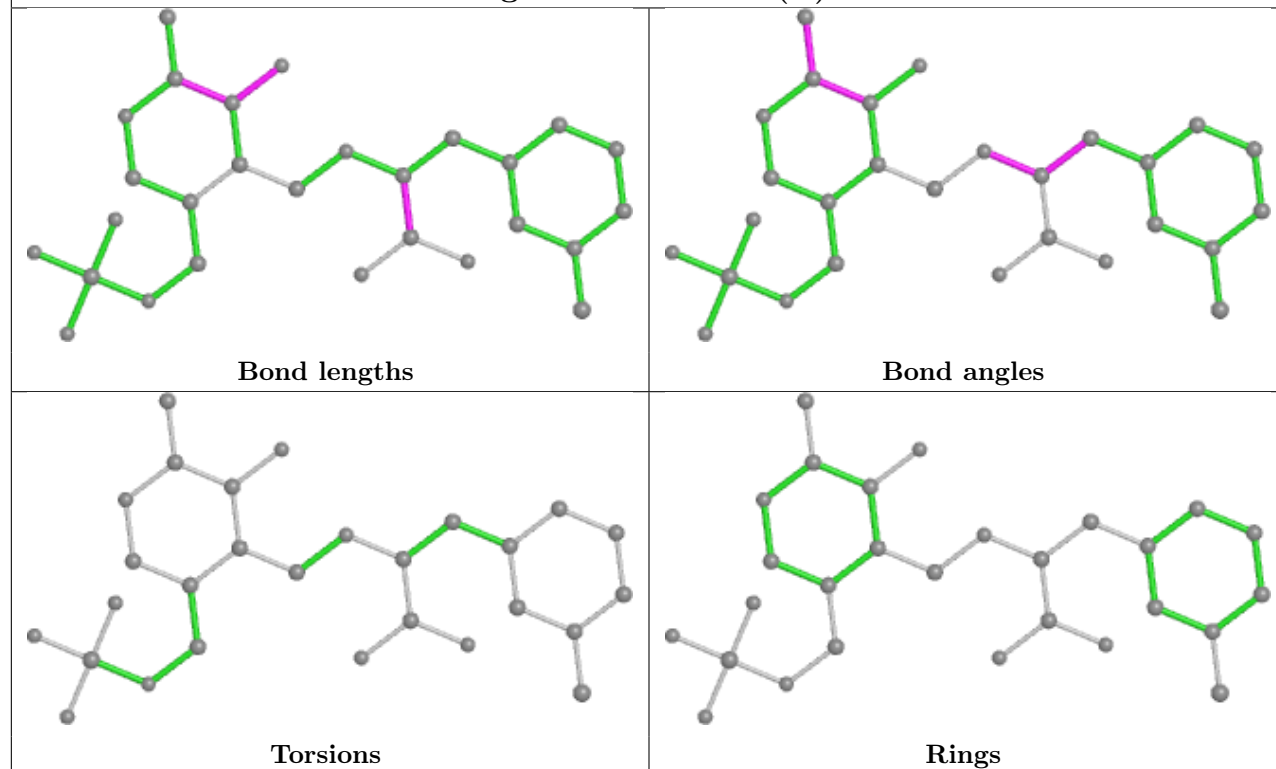
There are no ring outliers.

7 monomers are involved in 12 short contacts:

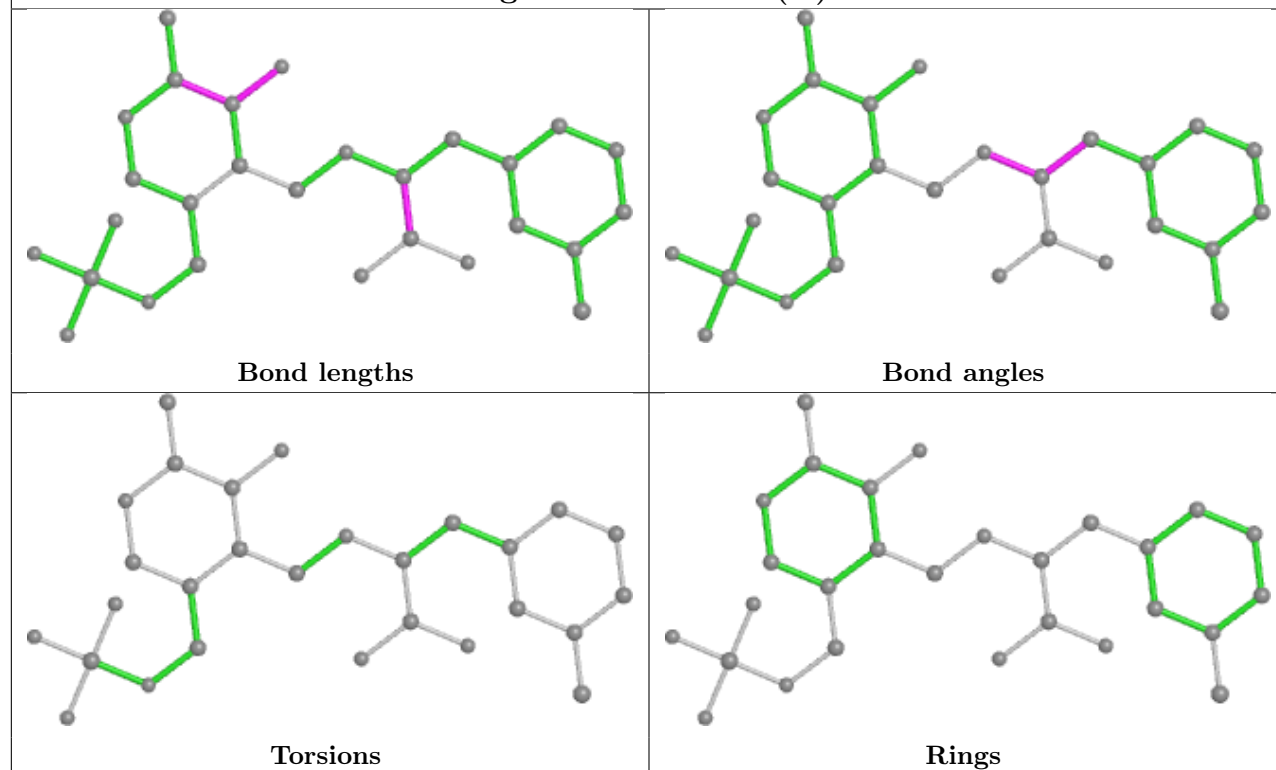
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	502[A]	PLP	1	0
3	A	501[B]	OY3	2	0
4	D	501	DMS	1	0
3	A	501[A]	OY3	4	0
6	C	502	PLP	1	0
3	B	501[B]	OY3	1	0
6	D	502	PLP	2	0

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.

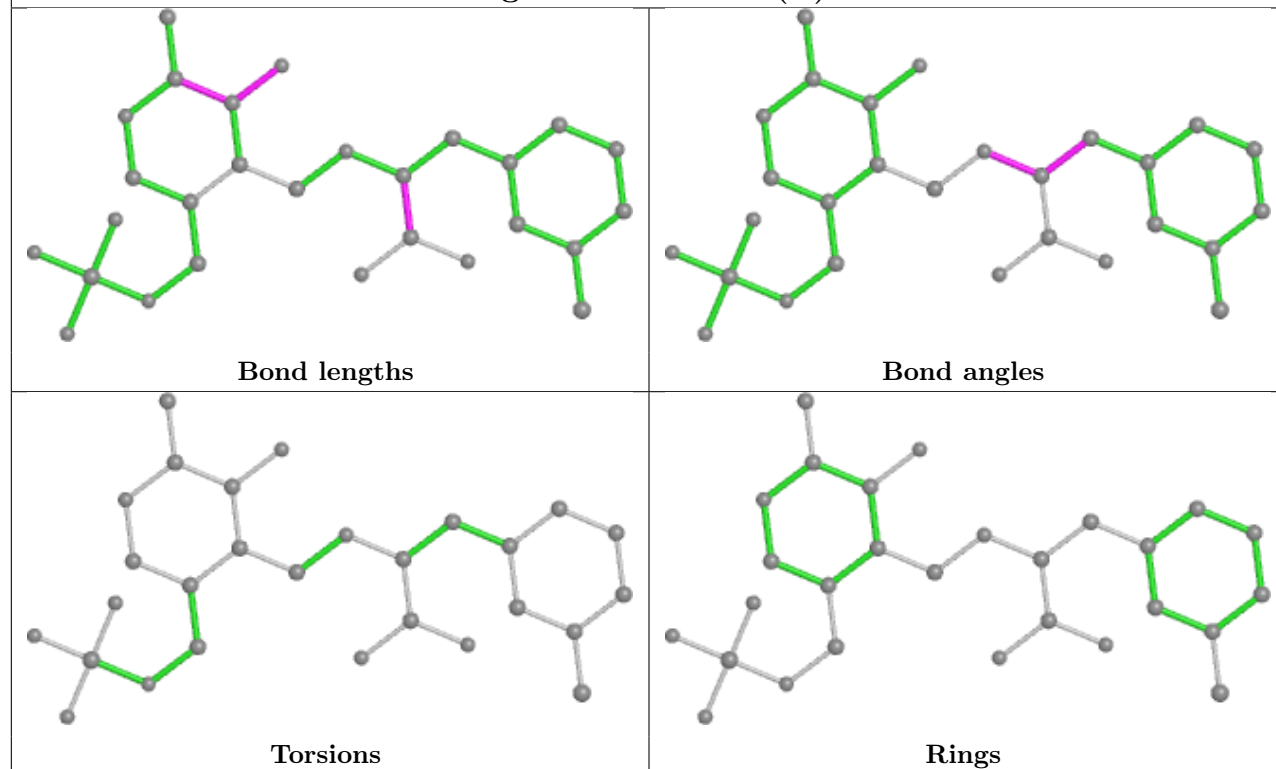
## Ligand OY3 A 501 (B)



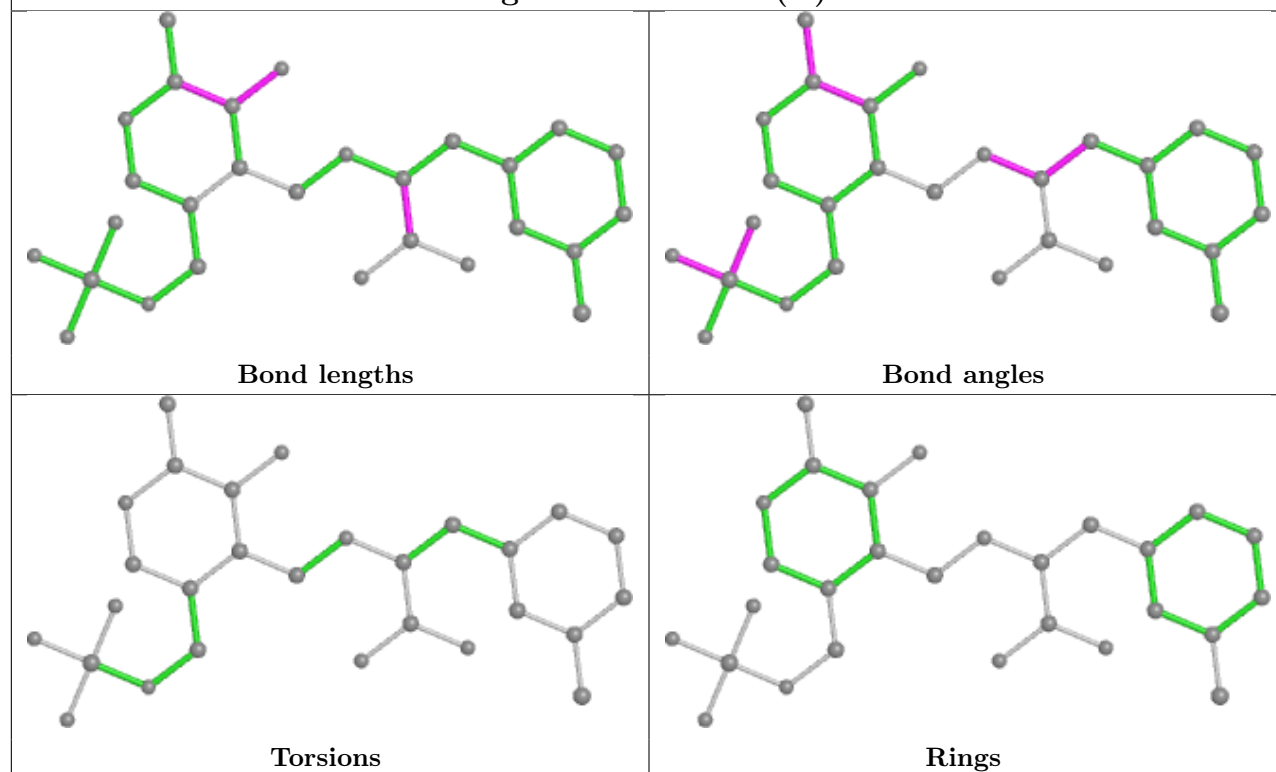
## Ligand OY3 A 501 (A)



## Ligand OY3 B 501 (B)



## Ligand OY3 B 501 (C)



## 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	456/456 (100%)	-0.02	21 (4%) 32 29	19, 32, 67, 107	0
1	B	456/456 (100%)	0.05	12 (2%) 56 53	21, 38, 68, 130	0
1	C	456/456 (100%)	-0.32	2 (0%) 92 92	18, 27, 42, 88	0
1	D	456/456 (100%)	-0.36	3 (0%) 87 87	19, 30, 47, 103	0
All	All	1824/1824 (100%)	-0.16	38 (2%) 63 62	18, 30, 61, 130	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	391	VAL	9.2
1	B	390	ASN	8.9
1	D	1	MET	8.0
1	A	391	VAL	5.2
1	A	456	ILE	5.2
1	A	390	ASN	3.8
1	B	393	GLY	3.8
1	A	1	MET	3.8
1	A	449	PHE	3.6
1	C	391	VAL	3.5
1	A	446	LEU	3.4
1	A	389	ASN	3.3
1	C	390	ASN	3.2
1	A	383	ILE	3.2
1	A	455	TYR	3.1
1	A	444	LYS	3.1
1	D	391[A]	VAL	2.9
1	B	389	ASN	2.8
1	A	393	GLY	2.7
1	A	396	HIS	2.7
1	D	456	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	444	LYS	2.6
1	A	357[A]	THR	2.5
1	A	443	PRO	2.3
1	A	448	PHE	2.3
1	A	453	PHE	2.3
1	B	392	THR	2.3
1	A	439	PHE	2.3
1	A	441	TYR	2.2
1	B	119	GLY	2.2
1	B	397	ARG	2.2
1	A	437	LEU	2.1
1	B	399	LYS	2.1
1	A	2	ASN	2.1
1	B	396	HIS	2.1
1	A	397	ARG	2.1
1	B	387	GLY	2.1
1	B	456	ILE	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no 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
4	DMS	A	504	4/4	0.88	0.19	41,73,76,76	0
4	DMS	D	501	4/4	0.90	0.14	25,30,37,41	0
4	DMS	C	504	4/4	0.93	0.13	33,40,51,52	0
3	OY3	B	501[C]	28/28	0.94	0.18	28,42,56,77	43
3	OY3	B	501[B]	28/28	0.94	0.18	28,42,55,61	43
4	DMS	C	503	4/4	0.95	0.08	27,33,35,35	0

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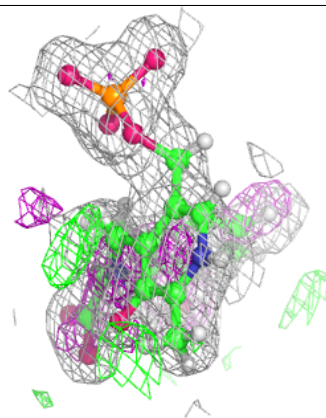
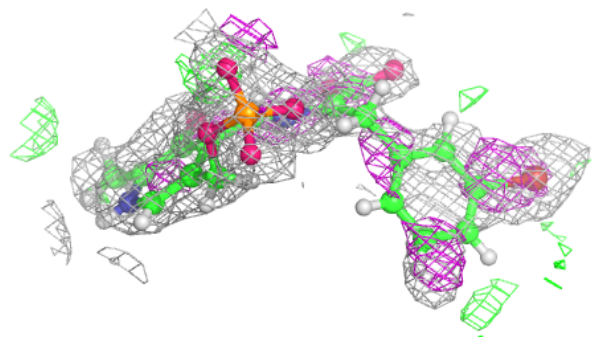
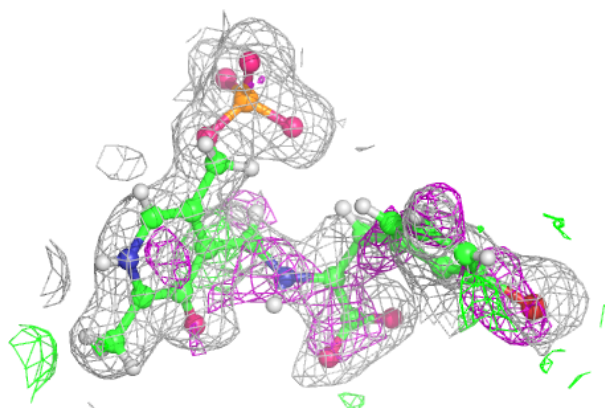
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OY3	A	501[B]	28/28	0.95	0.11	24,35,50,56	43
3	OY3	A	501[A]	28/28	0.95	0.11	24,35,50,58	43
6	PLP	B	502[A]	15/16	0.97	0.10	28,36,44,44	23
6	PLP	C	502	15/16	0.97	0.09	21,24,30,32	0
5	CL	D	503	1/1	0.98	0.04	34,34,34,34	0
6	PLP	D	502	15/16	0.98	0.08	23,26,31,36	0
5	CL	A	505	1/1	0.99	0.03	41,41,41,41	0
5	CL	C	501	1/1	0.99	0.04	34,34,34,34	0
2	K	C	505	1/1	1.00	0.05	20,20,20,20	0
2	K	C	506	1/1	1.00	0.06	21,21,21,21	0
2	K	A	502	1/1	1.00	0.07	22,22,22,22	0
2	K	A	503	1/1	1.00	0.06	22,22,22,22	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.

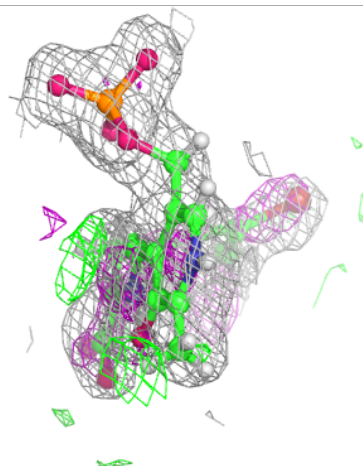
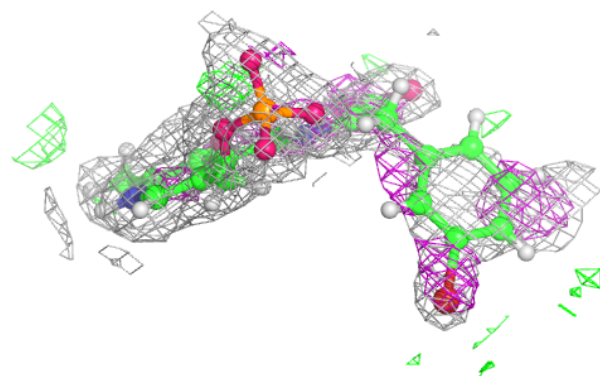
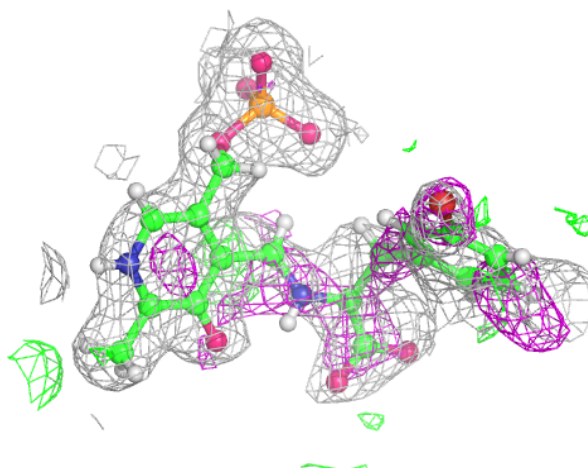
**Electron density around OY3 B 501 (C):**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around OY3 B 501 (B):**

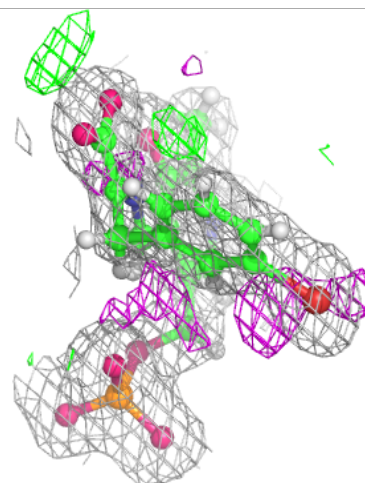
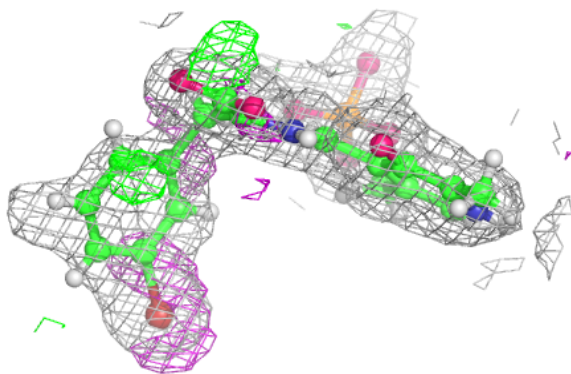
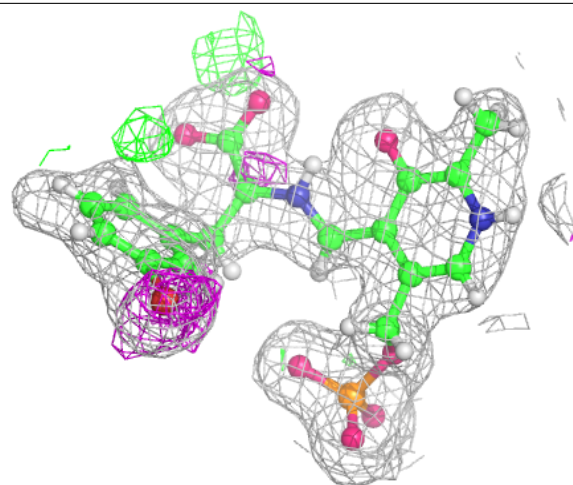
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





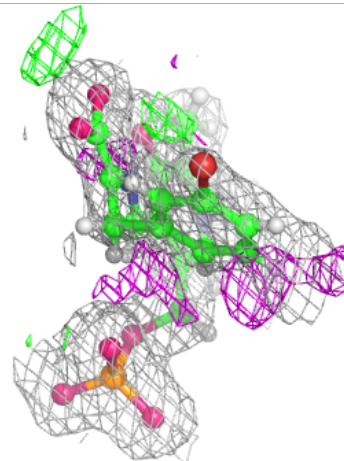
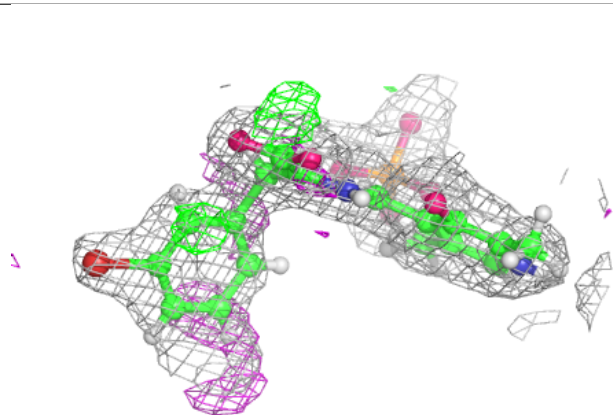
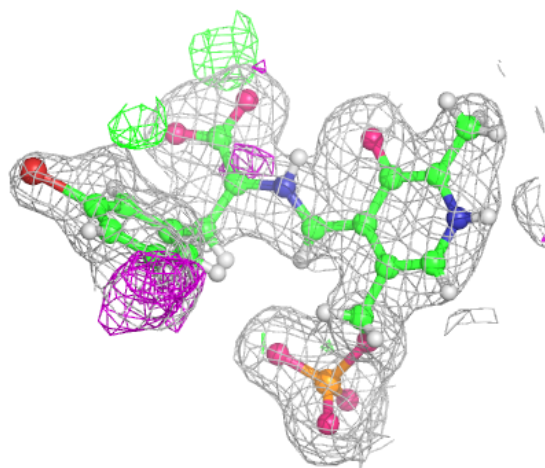
**Electron density around OY3 A 501 (B):**

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



**Electron density around OY3 A 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.