

### Full wwPDB X-ray Structure Validation Report (i)

### May 7, 2024 – 04:26 PM JST

PDB ID : 8K06

Title: Pseudouridine 5'-monophosphate glycosylase from Arabidopsis thaliana –

PSU, R5P bound K185A mutant

Authors: Lee, J.Y.; Kim, S.H.; Rhee, S.K.

Deposited on : 2023-07-07

Resolution : 1.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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 : 2.36.2buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

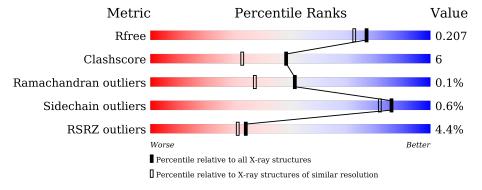
Validation Pipeline (wwPDB-VP) : 2.36.2

### 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.84 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	Similar resolution
WIGHT	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	340	79%	10%	11%
1	В	340	79%	10%	11%
1	С	340	77%	12%	11%



### 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7423 atoms, of which 20 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 Pseudouridine-5'-phosphate glycosidase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	303	Total	С	N	О	S	0	0	0
1	A	303	2229	1393	393	435	8	U	U	
1	D	204	Total	С	N	О	S	0	0	0
1	Ъ	304	2240	1399	397	436	8	0		
1	С	303	Total	С	N	О	S	0	0	0
1		303	2229	1393	393	435	8	0	U	

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	ALA	LYS	engineered mutation	UNP Q84K35
A	331	LEU	-	expression tag	UNP Q84K35
A	332	GLU	-	expression tag	UNP Q84K35
A	333	HIS	-	expression tag	UNP Q84K35
A	334	HIS	-	expression tag	UNP Q84K35
A	335	HIS	-	expression tag	UNP Q84K35
A	336	HIS	-	expression tag	UNP Q84K35
A	337	HIS	-	expression tag	UNP Q84K35
A	338	HIS	-	expression tag	UNP Q84K35
A	339	HIS	-	expression tag	UNP Q84K35
A	340	HIS	-	expression tag	UNP Q84K35
В	185	ALA	LYS	engineered mutation	UNP Q84K35
В	331	LEU	-	expression tag	UNP Q84K35
В	332	GLU	-	expression tag	UNP Q84K35
В	333	HIS	-	expression tag	UNP Q84K35
В	334	HIS	-	expression tag	UNP Q84K35
В	335	HIS	-	expression tag	UNP Q84K35
В	336	HIS	-	expression tag	UNP Q84K35
В	337	HIS	-	expression tag	UNP Q84K35
В	338	HIS	-	expression tag	UNP Q84K35
В	339	HIS	-	expression tag	UNP Q84K35
В	340	HIS	-	expression tag	UNP Q84K35
С	185	ALA	LYS	engineered mutation	UNP Q84K35



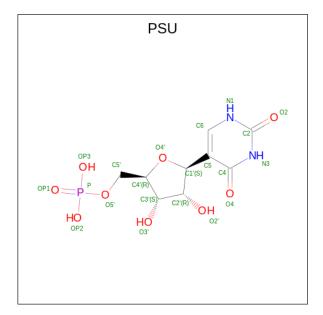
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Chain	Residue	Modelled	Actual	Comment	Reference
С	331	LEU	-	expression tag	UNP Q84K35
С	332	GLU	-	expression tag	UNP Q84K35
С	333	HIS	-	expression tag	UNP Q84K35
С	334	HIS	-	expression tag	UNP Q84K35
С	335	HIS	-	expression tag	UNP Q84K35
С	336	HIS	-	expression tag	UNP Q84K35
С	337	HIS	-	expression tag	UNP Q84K35
С	338	HIS	-	expression tag	UNP Q84K35
С	339	HIS	-	expression tag	UNP Q84K35
С	340	HIS	-	expression tag	UNP Q84K35

• Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	В	1	Total Mn 1 1	0	0
2	С	1	Total Mn 1 1	0	0

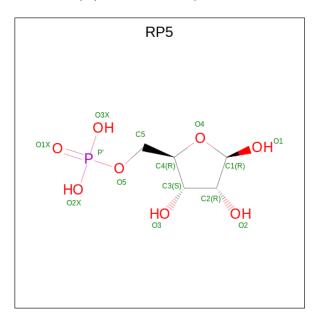
• Molecule 3 is PSEUDOURIDINE-5'-MONOPHOSPHATE (three-letter code: PSU) (formula:  $C_9H_{13}N_2O_9P$ ) (labeled as "Ligand of Interest" by depositor).





$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 21 9 2 9 1	0	0
3	С	1	Total C H N O P 32 9 11 2 9 1	0	0

• Molecule 4 is 5-O-phosphono-beta-D-ribofuranose (three-letter code: RP5) (formula:  $C_5H_{11}O_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
1	R	1	Total	С	Н	О	Р	0	0
4	В	1	23	5	9	8	1		

• Molecule 5 is water.

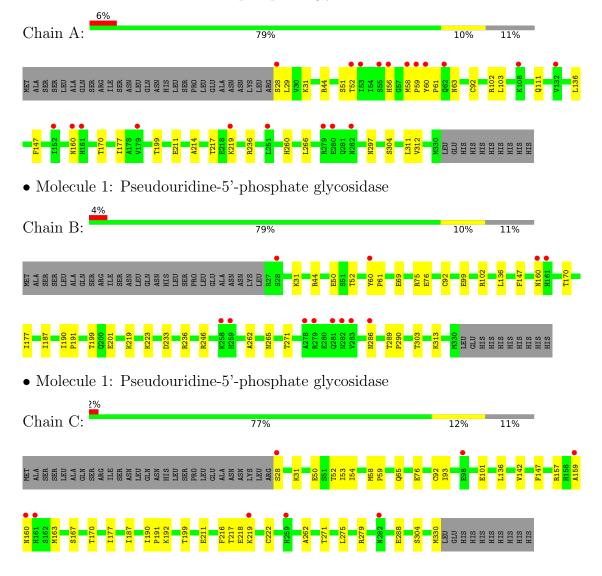
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	205	Total O 205 205	0	0
5	В	217	Total O 217 217	0	0
5	С	224	Total O 224 224	0	0



### 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: Pseudouridine-5'-phosphate glycosidase





### 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	72.56Å 105.84Å 73.56Å	Donogiton
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $118.87^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	29.92 - 1.84	Depositor
Resolution (A)	29.92 - 1.85	EDS
% Data completeness	97.6 (29.92-1.84)	Depositor
(in resolution range)	97.6 (29.92-1.85)	EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.37 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
$R, R_{free}$	0.182 , $0.208$	Depositor
it, it free	0.184 , $0.207$	DCC
$R_{free}$ test set	2033 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	$0.41 \; ,  54.1$	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.50, < L^2> = 0.34$	Xtriage
	0.002 for -h-l,k,h	
	0.002  for  l,k,-h-l	
Estimated twinning fraction	0.016  for h,-k,-h-l	Xtriage
	0.017  for -h-l,-k,l	
	0.017 for l,-k,h	
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7423	wwPDB-VP
Average B, all atoms $(\mathring{A}^2)$	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

### 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: RP5, PSU, MN

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		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.43	0/2259	0.55	0/3070	
1	В	0.44	0/2270	0.60	2/3084 (0.1%)	
1	С	0.44	0/2259	0.54	0/3070	
All	All	0.44	0/6788	0.56	2/9224 (0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	В	60	TYR	C-N-CD	7.97	145.14	128.40
1	В	60	TYR	C-N-CA	-5.33	99.62	122.00

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	2229	0	2275	26	0
1	В	2240	0	2288	29	0
1	С	2229	0	2275	31	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	21	0	11	0	0
3	С	21	11	11	1	0
4	В	14	9	0	0	0
5	A	205	0	0	8	0
5	В	217	0	0	13	2
5	С	224	0	0	9	2
All	All	7403	20	6860	81	2

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 (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
1 1 222 1 7 6 1112	- 1 - 201 TTOTT 0	distance (Å)	overlap (Å)
1:A:236:ARG:NH2	5:A:501:HOH:O	1.93	0.98
1:B:246:ARG:NH2	5:B:501:HOH:O	1.81	0.89
1:B:136:LEU:HD22	1:B:177:ILE:HG21	1.57	0.87
1:B:102:ARG:NH1	5:B:503:HOH:O	2.07	0.86
1:C:218:GLU:HG3	1:C:219:LYS:HG3	1.61	0.82
1:B:76:GLU:OE1	5:B:502:HOH:O	1.97	0.82
1:C:330:MET:O	5:C:501:HOH:O	1.99	0.79
1:A:136:LEU:HD22	1:A:177:ILE:HG21	1.64	0.78
1:C:136:LEU:HD22	1:C:177:ILE:HG21	1.66	0.77
1:B:265:ASN:ND2	1:B:303:THR:HG21	1.99	0.77
1:A:160:ASN:O	1:C:160:ASN:ND2	2.19	0.76
1:C:101:GLU:OE1	5:C:502:HOH:O	2.04	0.74
1:C:288:GLU:OE2	5:C:503:HOH:O	2.05	0.73
1:C:279:ARG:NH2	5:C:504:HOH:O	2.11	0.73
1:B:136:LEU:HD22	1:B:177:ILE:CG2	2.20	0.70
1:C:50:GLU:OE1	1:C:52:THR:HG22	1.92	0.70
1:B:265:ASN:CG	1:B:303:THR:HG21	2.14	0.68
1:A:136:LEU:HD22	1:A:177:ILE:CG2	2.25	0.67
1:B:136:LEU:CD2	1:B:177:ILE:HG21	2.26	0.65
1:A:58:MET:HB2	1:A:59:PRO:HD2	1.79	0.65
1:B:99:GLU:OE2	5:B:504:HOH:O	2.15	0.64
1:C:136:LEU:CD2	1:C:177:ILE:HG21	2.27	0.64
1:C:217:THR:HG22	1:C:262:ALA:O	1.98	0.63
1:C:136:LEU:HD22	1:C:177:ILE:CG2	2.28	0.63
1:B:50:GLU:OE1	1:B:52:THR:OG1	2.17	0.62
1:B:246:ARG:NE	5:B:501:HOH:O	2.31	0.60
1:C:211:GLU:OE1	1:C:219:LYS:NZ	2.34	0.60



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Continued from previous		Interatomic	Clash
Atom-1	Atom-2	${\rm distance}\ (\mathring{\rm A})$	overlap (Å)
1:B:44:ARG:NH1	5:B:509:HOH:O	2.33	0.60
1:C:65:GLN:HG2	5:C:695:HOH:O	2.01	0.60
1:A:29:LEU:HD11	5:A:536:HOH:O	2.03	0.57
1:B:160:ASN:ND2	5:B:511:HOH:O	2.37	0.57
1:A:111:GLN:HB3	5:A:520:HOH:O	2.04	0.57
1:C:31:LYS:NZ	1:C:92:CYS:SG	2.68	0.57
1:C:190:ILE:HB	1:C:191:PRO:HD3	1.87	0.57
1:B:75:ARG:HD3	5:B:510:HOH:O	2.05	0.56
1:A:260:HIS:HD2	5:A:672:HOH:O	1.87	0.56
1:A:51:SER:HB2	1:A:103:LEU:HD21	1.87	0.56
1:B:69:GLU:OE1	1:B:313:LYS:NZ	2.39	0.53
1:A:28:SER:OG	1:A:29:LEU:N	2.39	0.53
1:A:60:TYR:HA	1:A:63:ASN:OD1	2.09	0.52
1:C:76:GLU:HB2	5:C:509:HOH:O	2.09	0.52
1:C:58:MET:HB2	1:C:59:PRO:HD2	1.92	0.52
1:A:211:GLU:OE1	1:A:219:LYS:NZ	2.37	0.51
1:A:136:LEU:CD2	1:A:177:ILE:HG21	2.36	0.51
1:A:60:TYR:CE1	1:A:61:PRO:HB3	2.46	0.50
1:B:289:THR:HB	1:B:290:PRO:HD3	1.93	0.50
1:A:266:LEU:O	1:A:266:LEU:HD23	2.11	0.49
1:C:53:ILE:HD12	1:C:54:ILE:N	2.28	0.48
1:A:214:ALA:HB3	1:A:217:THR:HG23	1.96	0.48
1:C:93:ILE:HD12	1:C:142:VAL:HG11	1.94	0.48
1:C:159:ALA:O	1:C:163:MET:N	2.36	0.48
1:C:53:ILE:HD12	1:C:54:ILE:HG13	1.96	0.47
1:B:199:THR:HG22	1:C:170:THR:HG21	1.96	0.47
1:B:223:LYS:CE	5:B:505:HOH:O	2.62	0.47
1:B:246:ARG:CZ	5:B:501:HOH:O	2.36	0.46
1:B:31:LYS:NZ	1:B:92:CYS:SG	2.72	0.45
1:B:262:ALA:HA	1:B:265:ASN:HD22	1.82	0.45
1:B:233:ASP:OD1	1:B:236:ARG:NH2	2.33	0.44
1:C:222:CYS:SG	5:C:718:HOH:O	2.61	0.44
1:B:286:ASN:O	5:B:506:HOH:O	2.21	0.44
1:A:311:LEU:HD12	1:A:312:VAL:N	2.33	0.44
1:A:31:LYS:NZ	1:A:92:CYS:SG	2.71	0.44
1:A:297:ASN:HA	1:A:304:SER:OG	2.17	0.44
1:A:170:THR:HG21	1:C:199:THR:HG22	2.00	0.43
1:A:102:ARG:NE	5:A:502:HOH:O	2.15	0.43
1:C:28:SER:N	5:C:526:HOH:O	2.51	0.43
1:C:157:ARG:HD2	1:C:275:LEU:CD1	2.49	0.43
1:B:102:ARG:HD3	5:B:548:HOH:O	2.20	0.42



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0 0 1000100000			

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
1:B:190:ILE:HB	1:B:191:PRO:HD3	2.01	0.42
1:A:52:THR:O	1:A:56:HIS:N	2.45	0.42
1:B:201:GLU:HG2	1:C:167:SER:HB2	2.01	0.42
1:B:187:ILE:HG22	1:B:271:THR:HG23	2.01	0.42
1:A:102:ARG:HD2	5:A:617:HOH:O	2.19	0.41
1:A:111:GLN:NE2	5:A:523:HOH:O	2.51	0.41
1:B:160:ASN:CG	5:B:511:HOH:O	2.59	0.41
1:C:216:PHE:CE1	1:C:304:SER:HB2	2.55	0.41
1:C:52:THR:HG21	3:C:401:PSU:H1'	2.02	0.41
1:C:192:LYS:HD3	5:C:510:HOH:O	2.22	0.40
1:A:44:ARG:HD2	5:A:596:HOH:O	2.22	0.40
1:A:199:THR:HG22	1:B:170:THR:HG21	2.03	0.40
1:C:187:ILE:HG22	1:C:271:THR:HG23	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
5:B:641:HOH:O	5:C:648:HOH:O[1_455]	1.94	0.26
5:B:702:HOH:O	5:C:656:HOH:O[2_544]	1.98	0.22

### 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	Perce	entiles
1	A	301/340 (88%)	296 (98%)	5 (2%)	0	100	100
1	В	302/340 (89%)	297 (98%)	4 (1%)	1 (0%)	41	27
1	С	301/340 (88%)	297 (99%)	4 (1%)	0	100	100
All	All	904/1020 (89%)	890 (98%)	13 (1%)	1 (0%)	51	37

### All (1) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	61	PRO

### 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	240/274~(88%)	239 (100%)	1 (0%)	91 88
1	В	241/274 (88%)	239 (99%)	2 (1%)	81 75
1	С	240/274 (88%)	239 (100%)	1 (0%)	91 88
All	All	721/822 (88%)	717 (99%)	4 (1%)	86 82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	PHE
1	В	147	PHE
1	В	219	LYS
1	С	147	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	265	ASN
1	С	160	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)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	Trino	Chain	ain Res	Res Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	RP5	В	401	-	14,14,14	1.54	3 (21%)	20,21,21	1.78	4 (20%)
3	PSU	С	401	-	22,22,22	3.16	5 (22%)	29,33,33	1.64	4 (13%)
3	PSU	A	401	-	22,22,22	3.33	6 (27%)	29,33,33	1.74	5 (17%)

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
4	RP5	В	401	-	-	6/6/22/22	0/1/1/1
3	PSU	С	401	-	-	1/10/26/26	0/2/2/2
3	PSU	A	401	-	-	0/10/26/26	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
3	A	401	PSU	C6-C5	9.80	1.46	1.35
3	С	401	PSU	C6-C5	9.60	1.46	1.35
3	A	401	PSU	C2-N1	8.11	1.47	1.36
3	С	401	PSU	C2-N1	7.77	1.47	1.36
3	A	401	PSU	C2-N3	6.87	1.49	1.37
3	С	401	PSU	C2-N3	5.97	1.47	1.37
3	A	401	PSU	C6-N1	3.33	1.41	1.36
3	С	401	PSU	C6-N1	3.25	1.41	1.36



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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
4	В	401	RP5	O4-C1	2.74	1.46	1.43
3	A	401	PSU	C1'-C5	-2.69	1.44	1.50
4	В	401	RP5	C1-C2	-2.65	1.49	1.52
3	A	401	PSU	C4-N3	2.60	1.43	1.38
3	С	401	PSU	C1'-C5	-2.36	1.44	1.50
4	В	401	RP5	P'-O3X	-2.04	1.47	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
4	В	401	RP5	C1-C2-C3	4.88	108.41	102.30
3	С	401	PSU	C4-N3-C2	-4.60	119.71	126.34
3	С	401	PSU	N1-C2-N3	4.43	120.14	115.13
3	A	401	PSU	C4-N3-C2	-4.28	120.17	126.34
3	A	401	PSU	N1-C2-N3	4.14	119.82	115.13
3	A	401	PSU	O2-C2-N1	-3.85	118.55	122.79
4	В	401	RP5	O2X-P'-O5	3.77	116.75	106.73
3	A	401	PSU	C6-N1-C2	-3.37	119.24	122.68
3	A	401	PSU	C6-C5-C4	3.11	120.37	118.20
3	С	401	PSU	C6-N1-C2	-3.06	119.56	122.68
4	В	401	RP5	O5-P'-O1X	2.54	113.61	106.47
4	В	401	RP5	O2X-P'-O1X	-2.50	100.88	110.68
3	С	401	PSU	OP2-P-OP1	2.46	120.31	110.68

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	В	401	RP5	O4-C4-C5-O5
4	В	401	RP5	C5-O5-P'-O1X
4	В	401	RP5	C5-O5-P'-O2X
4	В	401	RP5	C5-O5-P'-O3X
4	В	401	RP5	C3-C4-C5-O5
4	В	401	RP5	C4-C5-O5-P'
3	С	401	PSU	O4'-C1'-C5-C6

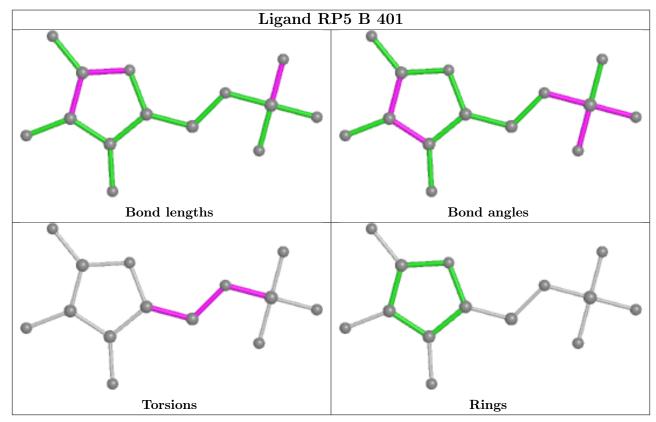
There are no ring outliers.

1 monomer is involved in 1 short contact:

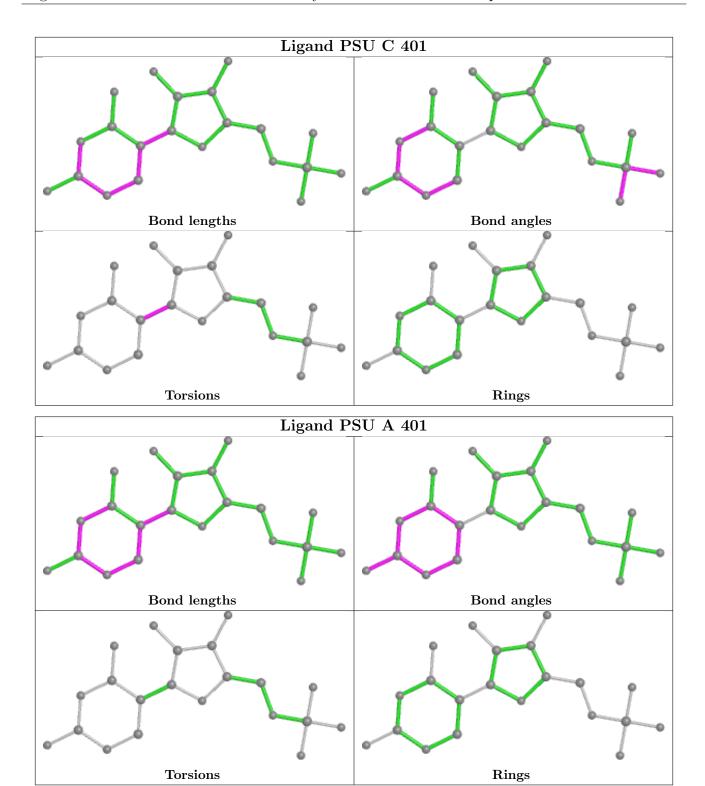
$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type	Clashes	Symm-Clashes
3	С	401	PSU	1	0



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 then 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ>2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	303/340 (89%)	0.21	20 (6%) 18 16	22, 30, 53, 69	0
1	В	304/340 (89%)	0.09	12 (3%) 39 36	21, 29, 49, 63	0
1	С	303/340 (89%)	0.02	8 (2%) 56 53	22, 31, 45, 58	0
All	All	910/1020 (89%)	0.11	40 (4%) 34 31	21, 30, 49, 69	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	PRO	7.1
1	A	53	ILE	7.1
1	С	160	ASN	5.6
1	A	56	HIS	4.8
1	A	62	GLN	4.7
1	В	161	HIS	4.5
1	В	282	ASN	4.1
1	В	279	ARG	4.0
1	В	60	TYR	3.8
1	A	60	TYR	3.6
1	A	282	ASN	3.5
1	С	161	HIS	3.5
1	В	283	VAL	3.4
1	С	259	HIS	3.4
1	A	279	ARG	3.3
1	В	259	HIS	3.3
1	A	52	THR	3.3
1	A	161	HIS	3.2
1	В	286	ASN	3.2
1	A	55	SER	3.2
1	A	152	ILE	3.0
1	В	160	ASN	3.0
1	A	58	MET	2.9



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Mol	Chain	Res	Type	RSRZ
1	A	108	LYS	2.8
1	С	159	ALA	2.8
1	С	28	SER	2.8
1	A	179	VAL	2.8
1	A	280	GLU	2.7
1	С	282	ASN	2.7
1	В	258	LYS	2.7
1	A	132	VAL	2.7
1	A	160	ASN	2.5
1	A	28	SER	2.4
1	С	219	LYS	2.4
1	С	98	GLU	2.4
1	В	278	ALA	2.4
1	В	28	SER	2.2
1	В	281	GLN	2.2
1	A	219	LYS	2.1
1	A	251	LEU	2.1

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

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

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

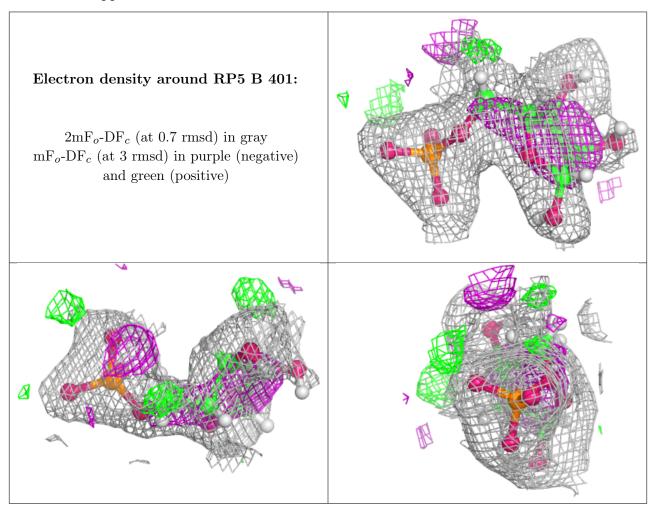
### 6.4 Ligands (i)

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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	RP5	В	401	14/14	0.91	0.17	33,52,63,71	0
3	PSU	С	401	21/21	0.93	0.12	33,48,58,61	0
3	PSU	A	401	21/21	0.93	0.13	34,45,58,61	0
2	MN	В	400	1/1	0.96	0.17	55,55,55,55	0
2	MN	A	400	1/1	0.99	0.05	32,32,32,32	0
2	MN	С	400	1/1	1.00	0.02	33,33,33,33	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 PSU A 401: $2mF_o$ -DF $_c$ (at 0.7 rmsd) in gray $mF_o$ -DF $_c$ (at 3 rmsd) in purple (negative) and green (positive)

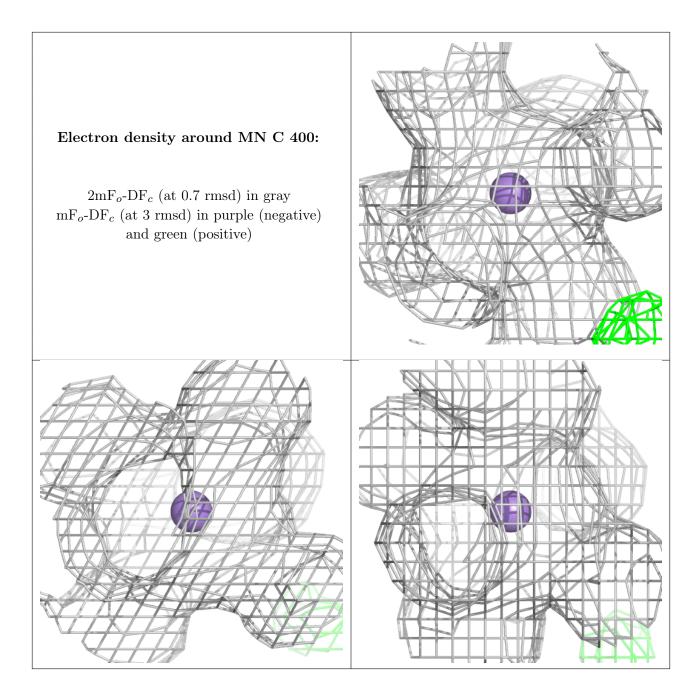


## Electron density around MN B 400: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



## Electron density around MN A 400: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





### 6.5 Other polymers (i)

There are no such residues in this entry.

