

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

#### May 14, 2020 – 07:11 pm BST

PDB ID : 5A30

Title: Crystal structure of mtPAP N472D mutant in complex with ATPgammaS

Authors : Lapkouski, M.; Hallberg, B.M.

Deposited on : 2015-05-26

Resolution : 2.75 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 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 : 2.11

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)

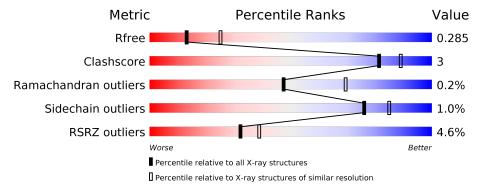
Validation Pipeline (wwPDB-VP) : 2.11

## 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 2.75 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 on 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	555	5% 77%	<b>%</b>	17%
1	В	555	78% 5	%	16%



## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7366 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 MITOCHONDRIAL PROTEIN.

$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	463	${ m Total} \ 3650$	C 2348	N 600	O 680	S 22	0	2	0
1	В	464	Total 3647	C 2351	N 595	O 680	S 21	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	expression tag	UNP F1NBW0
A	15	HIS	- expression tag		UNP F1NBW0
A	16	HIS	-	expression tag	UNP F1NBW0
A	17	HIS	-	expression tag	UNP F1NBW0
A	18	HIS	-	expression tag	UNP F1NBW0
A	19	HIS	-	expression tag	UNP F1NBW0
A	20	HIS	-	expression tag	UNP F1NBW0
A	21	SER	_	expression tag	UNP F1NBW0
A	22	SER	_	expression tag	UNP F1NBW0
A	23	GLY	_	expression tag	UNP F1NBW0
A	24	VAL	_	expression tag	UNP F1NBW0
A	25	ASP	_	expression tag	UNP F1NBW0
A	26	LEU	_	expression tag	UNP F1NBW0
A	27	GLY	_	expression tag	UNP F1NBW0
A	28	THR	-	expression tag	UNP F1NBW0
A	29	GLU	_	expression tag	UNP F1NBW0
A	30	ASN	-	expression tag	UNP F1NBW0
A	31	LEU	_	expression tag	UNP F1NBW0
A	32	TYR	_	expression tag	UNP F1NBW0
A	33	PHE	_	expression tag	UNP F1NBW0
A	34	GLN	_	expression tag	UNP F1NBW0
A	35	SER	-	expression tag	UNP F1NBW0
A	36	MET	-	expression tag	UNP F1NBW0
A	472	ASP	ASN	engineered mutation	UNP F1NBW0
В	14	MET	-	expression tag	UNP F1NBW0



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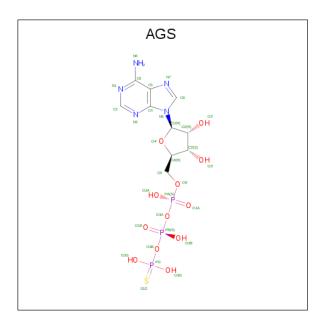
Chain	Residue	Modelled	Actual	Comment	Reference
В	15	HIS	-	expression tag	UNP F1NBW0
В	16	HIS	_	expression tag	UNP F1NBW0
В	17	HIS	_	expression tag	UNP F1NBW0
В	18	HIS	_	expression tag	UNP F1NBW0
В	19	HIS	-	expression tag	UNP F1NBW0
В	20	HIS	-	expression tag	UNP F1NBW0
В	21	SER	-	expression tag	UNP F1NBW0
В	22	SER	_	expression tag	UNP F1NBW0
В	23	GLY	-	expression tag	UNP F1NBW0
В	24	VAL	-	expression tag	UNP F1NBW0
В	25	ASP	_	expression tag	UNP F1NBW0
В	26	LEU	-	expression tag	UNP F1NBW0
В	27	GLY	_	expression tag	UNP F1NBW0
В	28	THR	_	expression tag	UNP F1NBW0
В	29	GLU	-	expression tag	UNP F1NBW0
В	30	ASN	_	expression tag	UNP F1NBW0
В	31	LEU	_	expression tag	UNP F1NBW0
В	32	TYR	_	expression tag	UNP F1NBW0
В	33	PHE	_	expression tag	UNP F1NBW0
В	34	GLN	-	expression tag	UNP F1NBW0
В	35	SER	-	expression tag	UNP F1NBW0
В	36	MET	-	expression tag	UNP F1NBW0
В	472	ASP	ASN	engineered mutation	UNP F1NBW0

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
2	В	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

• Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula:  $C_{10}H_{16}N_5O_{12}P_3S$ ).





Mol	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf			
9	Λ	1	Total	С	N	О	Р	S	0	0	
3	A	1	31	10	5	12	3	1	U	0	
9	D	1	Total	С	N	О	Р	S	0	0	
3	Б	1	31	10	5	12	3	1	U	U	

### • Molecule 4 is water.

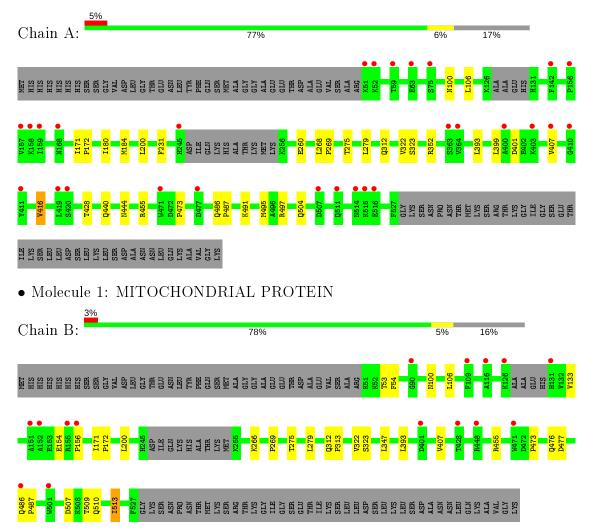
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total O 3 3	0	0
4	В	2	Total O 2 2	0	0



## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: MITOCHONDRIAL PROTEIN





# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	60.23Å 95.22Å 190.51Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	39.75 - 2.75	Depositor	
Resolution (A)	39.72 - 2.75	EDS	
% Data completeness	99.6 (39.75-2.75)	Depositor	
(in resolution range)	99.6 (39.72-2.75)	EDS	
$R_{merge}$	0.14	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	1.66 (at 2.77Å)	Xtriage	
Refinement program	REFMAC 5.7.0032	Depositor	
P. P.	0.247 , $0.287$	Depositor	
$R, R_{free}$	0.247 , $0.285$	DCC	
$R_{free}$ test set	1484 reflections $(5.09\%)$	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	66.7	Xtriage	
Anisotropy	0.376	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.33, 36.3	EDS	
L-test for twinning <sup>2</sup>	$ < L > = 0.47, < L^2> = 0.30$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
$F_o, F_c$ correlation	0.92	EDS	
Total number of atoms	7366	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.12% 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: MG, AGS

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	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5	
1	A	0.32	0/3743	0.51	1/5080~(0.0%)	
1	В	0.32	0/3734	0.52	0/5066	
All	All	0.32	0/7477	0.51	1/10146 (0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^o)$
1	A	416	VAL	CB-CA-C	-5.34	101.26	111.40

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	3650	0	3543	19	0
1	В	3647	0	3540	18	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
3	A	31	0	12	1	0
3	В	31	0	12	0	0
4	A	3	0	0	0	0
4	В	2	0	0	0	0



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$\mathbf{Mol}$	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
All	All	7366	0	7107	37	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 3.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 0 mg 1	A 4 0 mg 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance} \; ({ m \AA})$	$overlap(\AA)$
1:A:180:ILE:HG22	1:A:184:MET:CE	2.13	0.79
1:A:180:ILE:HG22	1:A:184:MET:HE2	1.66	0.77
1:A:231:PHE:O	1:A:352:ARG:NH2	2.29	0.65
1:B:154:GLU:C	1:B:156:PRO:HA	2.20	0.62
1:A:100:ASN:ND2	1:A:312:GLN:O	2.33	0.62
1:B:154:GLU:O	1:B:156:PRO:HA	2.01	0.60
1:B:100:ASN:ND2	1:B:312:GLN:O	2.34	0.60
1:B:507:ASP:OD2	1:B:510:GLN:HB2	2.04	0.57
1:B:455:ARG:NH1	1:B:473:PRO:O	2.42	0.52
1:A:399:LEU:HB2	1:A:416:VAL:CG2	2.40	0.51
1:B:476:GLN:O	1:B:477:ASP:HB2	2.10	0.50
1:A:455:ARG:NH1	1:A:473:PRO:O	2.42	0.50
1:B:486:GLN:HB3	1:B:487:PRO:HD3	1.97	0.47
1:A:486:GLN:HB3	1:A:487:PRO:HD3	1.97	0.47
1:B:393:LEU:HB3	1:B:455:ARG:HA	1.97	0.47
1:A:393:LEU:HB3	1:A:455:ARG:HA	1.97	0.46
1:A:444:ASN:OD1	1:A:497:ARG:NH1	2.44	0.46
1:B:171:ILE:HB	1:B:172:PRO:HD3	1.99	0.45
1:A:399:LEU:HB2	1:A:416:VAL:HG22	2.00	0.44
1:A:440[A]:GLN:OE1	1:A:504:GLN:NE2	2.49	0.43
1:A:275:THR:HG23	1:A:322:VAL:CG2	2.49	0.43
1:B:509:THR:O	1:B:513:ILE:HD13	2.19	0.43
1:B:322:VAL:HG12	1:B:323:SER:HB2	2.01	0.43
1:A:171:ILE:HB	1:A:172:PRO:HD3	2.01	0.42
1:A:279:LEU:HD11	1:A:322:VAL:HG23	2.01	0.42
1:B:154:GLU:O	1:B:156:PRO:CA	2.68	0.42
1:A:180:ILE:HG22	1:A:184:MET:HE3	1.97	0.42
3:A:1529:AGS:O2B	3:A:1529:AGS:H5'2	2.20	0.42
1:A:106:LEU:HD12	1:A:200:LEU:HD12	2.01	0.41
1:B:312:GLN:N	1:B:313:PRO:CD	2.82	0.41
1:A:268:LEU:HD21	1:B:133:VAL:HG22	2.02	0.41
1:B:106:LEU:HD12	1:B:200:LEU:HD12	2.02	0.41
1:B:279:LEU:HD11	1:B:322:VAL:HG23	2.02	0.41



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Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:A:322:VAL:HG12	1:A:323:SER:HB2	2.02	0.40
1:B:53:THR:O	1:B:54:PHE:C	2.59	0.40
1:A:491:LYS:O	1:A:495:MET:HG2	2.21	0.40
1:B:275:THR:HG23	1:B:322:VAL:CG2	2.51	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	Percen	tiles
1	A	459/555~(83%)	441 (96%)	17 (4%)	1 (0%)	47	69
1	В	458/555 $(82%)$	441 (96%)	16 (4%)	1 (0%)	47	69
All	All	917/1110 (83%)	882 (96%)	33 (4%)	2 (0%)	47	69

#### All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	269	PRO
1	A	269	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.



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		1 0			
Mol	Chain	${f Analy sed}$	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Analysed Rotameric C		Percentiles
1	A	401/497 (81%)	397 (99%)	4 (1%)	76 85
1	В	398/497 (80%)	394 (99%)	4 (1%)	76 85
All	All	799/994 (80%)	791 (99%)	8 (1%)	76 85

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	GLU
1	A	401	ASP
1	A	407	VAL
1	A	428	THR
1	В	266	LYS
1	В	347	LEU
1	В	407	VAL
1	В	513	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	GLN
1	A	511	GLN
1	В	312	GLN
1	В	510	GLN
1	В	511	GLN

#### 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 carbohydrates in this entry.



### 5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	Т	Chain	Res	Link	Во	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
3	AGS	В	1528	2	26,33,33	4.51	8 (30%)	26,52,52	2.16	4 (15%)	
3	AGS	A	1529	2	26,33,33	4.52	8 (30%)	26,52,52	2.23	4 (15%)	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	В	1528	2	-	1/17/38/38	0/3/3/3
3	AGS	A	1529	2	_	2/17/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}( ext{\AA})$
3	В	1528	AGS	O4'-C1'	15.40	1.62	1.41
3	A	1529	AGS	O4'-C1'	15.18	1.62	1.41
3	A	1529	AGS	C2'-C1'	-13.35	1.33	1.53
3	В	1528	AGS	C2'-C1'	-13.17	1.33	1.53
3	В	1528	AGS	O4'-C4'	-6.82	1.29	1.45
3	A	1529	AGS	O4'-C4'	-6.62	1.30	1.45
3	A	1529	AGS	C6-N6	3.95	1.48	1.34
3	В	1528	AGS	C6-N6	3.92	1.48	1.34
3	A	1529	AGS	O2'-C2'	3.55	1.51	1.43
3	A	1529	AGS	C2-N1	3.50	1.40	1.33
3	В	1528	AGS	O2'-C2'	3.46	1.51	1.43
3	A	1529	AGS	C2-N3	3.42	1.37	1.32
3	В	1528	AGS	C2-N1	3.00	1.39	1.33
3	В	1528	AGS	C2-N3	2.90	1.36	1.32
3	A	1529	AGS	PA-O1A	2.33	1.59	1.50
3	В	1528	AGS	PA-O1A	2.26	1.58	1.50



All (8) bond angle outliers are listed belo	All (	3) bond angle	outliers are	listed below
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$Ideal(^{o})$
3	A	1529	AGS	C5-C6-N6	7.33	131.49	120.35
3	В	1528	AGS	C5-C6-N6	6.89	130.82	120.35
3	В	1528	AGS	N3-C2-N1	-5.78	119.65	128.68
3	A	1529	AGS	N3-C2-N1	-5.55	120.01	128.68
3	A	1529	AGS	N6-C6-N1	-4.55	109.13	118.57
3	В	1528	AGS	N6-C6-N1	-4.35	109.54	118.57
3	В	1528	AGS	PA-O3A-PB	-2.42	124.52	132.83
3	A	1529	AGS	PA-O3A-PB	-2.21	125.23	132.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	1528	AGS	PA-O3A-PB-O2B
3	A	1529	AGS	PA-O3A-PB-O2B
3	A	1529	AGS	PA-O3A-PB-O1B

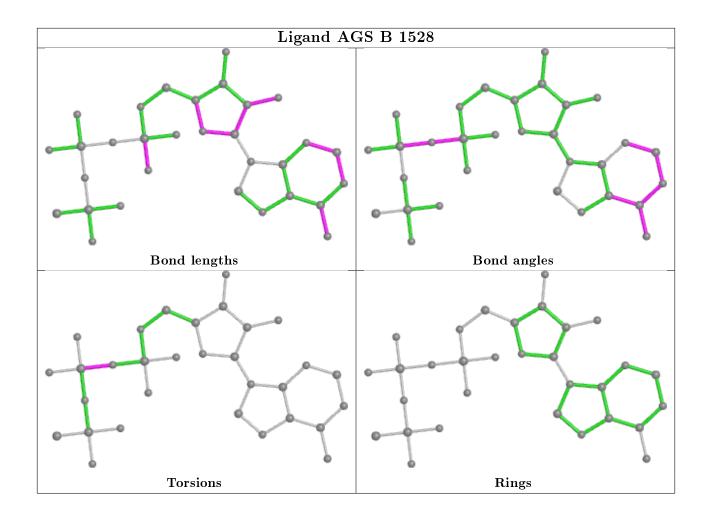
There are no ring outliers.

1 monomer is involved in 1 short contact:

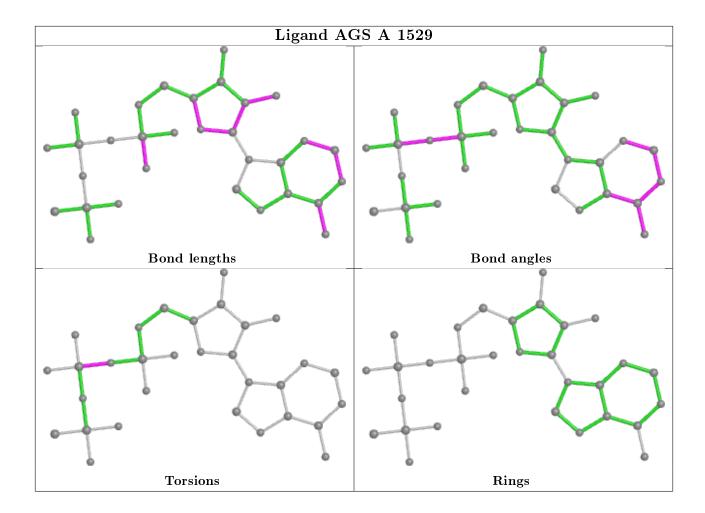
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1529	AGS	1	0

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 $>$	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	463/555 $(83%)$	0.44	28 (6%) 21 26	47, 71, 101, 124	0
1	В	464/555~(83%)	0.29	15 (3%) 47 56	44, 64, 95, 138	0
All	All	927/1110 (83%)	0.36	43 (4%) 32 39	44, 67, 99, 138	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	156	PRO	5.2
1	В	155	ARG	4.8
1	A	245	HIS	4.5
1	A	507	ASP	3.9
1	В	401	ASP	3.5
1	A	411	TYR	3.4
1	A	471	TRP	3.4
1	A	477	ASP	3.4
1	A	419	LEU	3.2
1	A	410	GLY	3.1
1	A	52	LYS	3.1
1	A	403	LYS	3.1
1	В	126	LYS	3.0
1	A	420	SER	2.9
1	A	407	VAL	2.9
1	A	363	SER	2.9
1	A	156	PRO	2.8
1	A	514	ASN	2.8
1	A	515	LYS	2.7
1	В	131	HIS	2.7
1	A	51	LYS	2.7
1	В	151	ALA	2.7
1	В	448	ARG	2.6
1	A	511	GLN	2.5



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Mol	Chain	Res	Type	RSRZ
1	В	116	ALA	2.5
1	В	428	THR	2.5
1	A	63	GLU	2.5
1	В	152	ALA	2.4
1	A	159	ILE	2.3
1	A	168	ASN	2.3
1	В	90	GLY	2.2
1	В	501	TRP	2.2
1	A	364	VAL	2.2
1	A	59	THR	2.2
1	A	400	ALA	2.2
1	A	157	VAL	2.1
1	A	158	LYS	2.1
1	A	142	PHE	2.1
1	A	516	GLU	2.1
1	В	471	TRP	2.1
1	В	486	GLN	2.1
1	A	75	SER	2.1
1	В	109	PHE	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 carbohydrates in this entry.

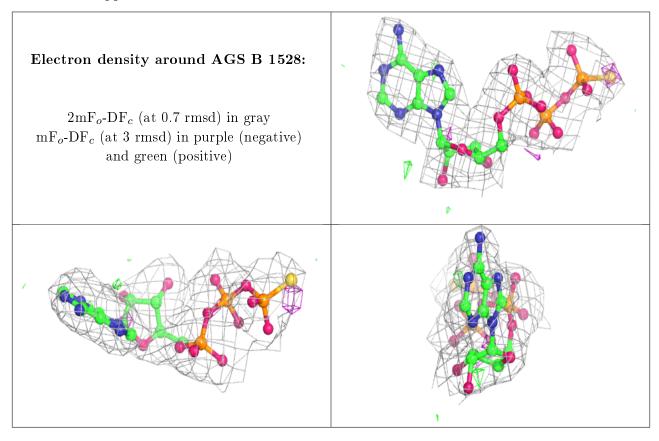
### 6.4 Ligands (i)

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.

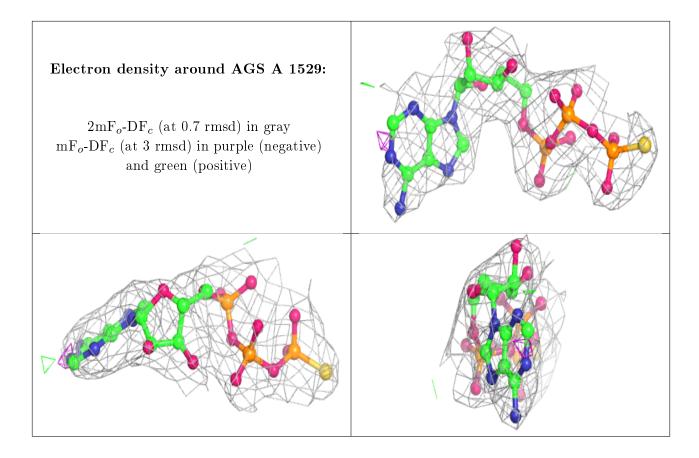
Mol	Type	Chain	$\operatorname{Res}$	Atoms	RSCC	RSR	$oxed{f B-factors({ m \AA}^2)}$	Q<0.9
3	AGS	В	1528	31/31	0.96	0.14	47,52,56,72	0
3	AGS	A	1529	31/31	0.96	0.14	51,64,72,75	0
2	MG	В	1529	1/1	0.96	0.12	43,43,43,43	0
2	MG	A	1528	1/1	0.97	0.14	59,59,59,59	0



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.







## 6.5 Other polymers (i)

There are no such residues in this entry.

