

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

Apr 9, 2022 – 10:19 pm BST

PDB ID	:	7070
Title	:	KRasG12C ligand complex
Authors	:	Phillips, C.
Deposited on	:	2021-04-12
Resolution	:	1.18  Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

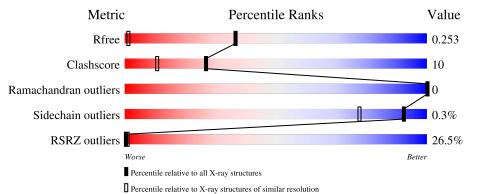
MolProbity		4 02b 467
•		
Mogul	:	1.8.4, CSD as $541$ be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.18 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1123 (1.20-1.16)
Clashscore	141614	1182 (1.20-1.16)
Ramachandran outliers	138981	1134 (1.20-1.16)
Sidechain outliers	138945	1134 (1.20-1.16)
RSRZ outliers	127900	1102 (1.20-1.16)

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	٨	170	26%					
	A	170	88%	11% •				
1	D	170	82%	16% ••				



## 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3182 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	168	Total	С	Ν	0	S	0	0	0
	A	108	1340	840	230	265	5	0		
1	л	168	Total	С	Ν	0	S	0	0	0
	I D	168	1340	840	230	265	5	0	0	0

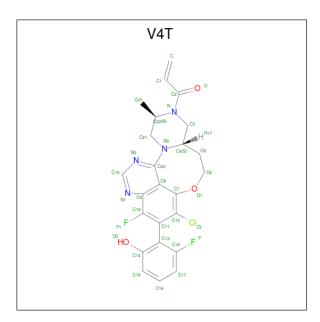
• Molecule 1 is a protein called GTPase KRas.

There are 10 discrepancies between the modelled and reference sequences:	
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Chain	Residue	Modelled	Actual Comment		Reference
А	0	GLY	-	expression tag	UNP P01116
А	12	CYS	GLY	engineered mutation	UNP P01116
А	51	SER	CYS	engineered mutation	UNP P01116
А	80	LEU	CYS	engineered mutation	UNP P01116
А	118	SER	CYS	engineered mutation	UNP P01116
D	0	GLY	-	expression tag	UNP P01116
D	12	CYS	GLY	engineered mutation	UNP P01116
D	51	SER	CYS	engineered mutation	UNP P01116
D	80	LEU	CYS	engineered mutation	UNP P01116
D	118	SER	CYS	engineered mutation	UNP P01116

• Molecule 2 is 1-[(4R,7S)-12-chloro-14-fluoro-13-(2-fluoro-6-hydroxyphenyl)-4-methyl-10-ox a-2,5,16,18-tetrazatetracyclo[9.7.1.0^(2,7).0^(15,19)]nonadeca-1(18),11,13,15(19),16-pen taen-5-en-1-one-yl]prop-2 (three-letter code: V4T) (formula:  $C_{24}H_{21}ClF_2N_4O_3$ ) (labeled as "Ligand of Interest" by depositor).





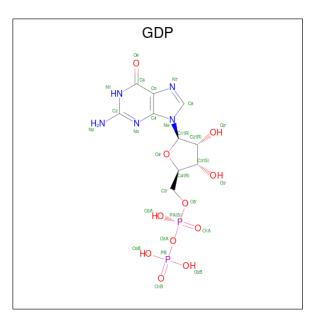
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
2	2 A	1	Total	С	Cl	F	Ν	0	0	0	
		1	34	24	1	2	4	3	0		
2	Л	1	Total	С	Cl	F	Ν	0	0	0	
	2 D	1	34	24	1	2	4	3	0	U	

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

• Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $\rm C_{10}H_{15}N_5O_{11}P_2).$ 





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	4 A	1	Total	С	Ν	Ο	Р	0	0
4		1	28	10	5	11	2	0	0
4	Л	1	Total	С	Ν	Ο	Р	0	0
4	4 D	1	28	10	5	11	2	0	U

• Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0

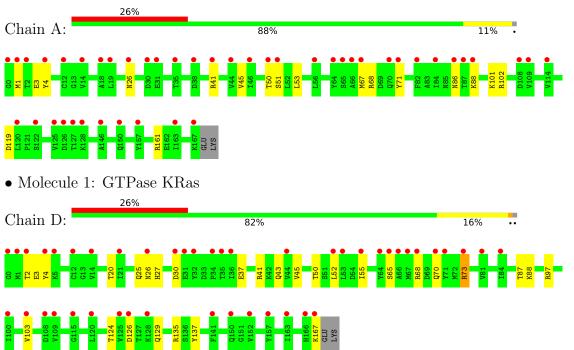
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	183	Total O 183 183	0	0
6	D	191	Total O 191 191	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: GTPase KRas



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	33.38Å 70.46Å 66.15Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.26^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	17.03 - 1.18	Depositor
Resolution (A)	17.02 - 1.18	EDS
% Data completeness	75.7(17.03-1.18)	Depositor
(in resolution range)	75.8 (17.02-1.18)	EDS
R <sub>merge</sub>	0.04	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$49.91 (at 1.18 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
$R, R_{free}$	0.226 , $0.257$	Depositor
II, II, <i>free</i>	0.225 , $0.253$	DCC
$R_{free}$ test set	3816 reflections $(5.07%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	12.0	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$< L >=0.58, < L^2>=0.44$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3182	wwPDB-VP
Average B, all atoms $(Å^2)$	17.0	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 56.89 % 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 2.5642e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;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.



<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: GDP, V4T, CA, MG  $\,$ 

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	Bond lengths		nd angles
Moi Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.81	0/1361	0.95	4/1836~(0.2%)
1	D	0.85	0/1361	1.05	4/1836~(0.2%)
All	All	0.83	0/2722	1.00	8/3672~(0.2%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	D	137	TYR	CB-CG-CD1	8.63	126.18	121.00
1	D	73	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	А	161	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	А	161	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	D	97	ARG	NE-CZ-NH1	-5.96	117.32	120.30

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	А	1340	0	1324	26	0
1	D	1340	0	1324	36	0
2	А	34	0	0	0	0
2	D	34	0	0	0	0

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Mol	*	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	А	1	0	0	0	0
3	D	1	0	0	0	0
4	А	28	0	12	0	0
4	D	28	0	12	1	0
5	А	1	0	0	0	0
5	D	1	0	0	0	0
6	А	183	0	0	11	0
6	D	191	0	0	13	1
All	All	3182	0	2672	56	1

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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 10.

The worst 5 of 56 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:86:ASN:CG	6:A:305:HOH:O	1.92	1.06
1:D:25:GLN:HE21	1:D:27:HIS:HE1	1.13	0.94
1:A:68:ARG:NE	6:A:301:HOH:O	2.03	0.91
1:D:26:ASN:HB3	6:D:457:HOH:O	1.71	0.88
1:D:68:ARG:NE	6:D:301:HOH:O	2.07	0.86

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
6:D:374:HOH:O	6:D:462:HOH:O[2_644]	2.07	0.13

### 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	ntiles
1	А	166/170~(98%)	161 (97%)	5(3%)	0	100	100
1	D	166/170~(98%)	164 (99%)	2(1%)	0	100	100
All	All	332/340~(98%)	325~(98%)	7(2%)	0	100	100

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Analysed Rotameric Outliers		Percentiles		
1	А	148/150~(99%)	148 (100%)	0	100 100		
1	D	148/150~(99%)	147~(99%)	1 (1%)	84 57		
All	All	296/300~(99%)	295 (100%)	1 (0%)	92 78		

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	167	LYS

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

Mol	Chain	Res	Type
1	А	43	GLN
1	А	129	GLN
1	D	27	HIS
1	D	43	GLN
1	D	129	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 monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	Turne	Chain Res Link		tes Link G Bond lengths			Bond angles								
	Type	Chain	nes	nes	nes	res 1	nes	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	V4T	D	201	1	37,38,38	1.26	4 (10%)	37,57,57	1.47	3 (8%)					
2	V4T	А	201	1	37,38,38	1.18	4 (10%)	37,57,57	1.80	5 (13%)					
4	GDP	D	203	3	24,30,30	1.33	5 (20%)	31,47,47	2.06	4 (12%)					
4	GDP	А	203	3	24,30,30	1.31	2 (8%)	31,47,47	1.72	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
2	V4T	D	201	1	-	2/10/36/36	0/4/5/5
2	V4T	А	201	1	-	2/10/36/36	0/4/5/5
4	GDP	D	203	3	-	2/12/32/32	0/3/3/3
4	GDP	А	203	3	-	1/12/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	V4T	O1-C6	-4.52	1.38	1.44

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Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(Å)	Ideal(Å)
2	А	201	V4T	C-C1	4.43	1.52	1.30
2	D	201	V4T	C-C1	4.08	1.50	1.30
4	А	203	GDP	C6-N1	4.05	1.40	1.33
4	D	203	GDP	C6-N1	3.29	1.38	1.33

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The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	D	203	GDP	C5-C6-N1	-7.72	112.87	123.43
4	А	203	GDP	C5-C6-N1	-6.31	114.80	123.43
2	А	201	V4T	O1-C7-C12	6.23	124.13	118.81
4	D	203	GDP	C2-N1-C6	5.88	125.28	115.93
2	А	201	V4T	C-C1-C2	-5.78	109.50	121.33

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	203	GDP	PA-O3A-PB-O3B
4	D	203	GDP	PA-O3A-PB-O1B
2	А	201	V4T	C-C1-C2-N
4	D	203	GDP	PA-O3A-PB-O3B
2	А	201	V4T	C-C1-C2-O

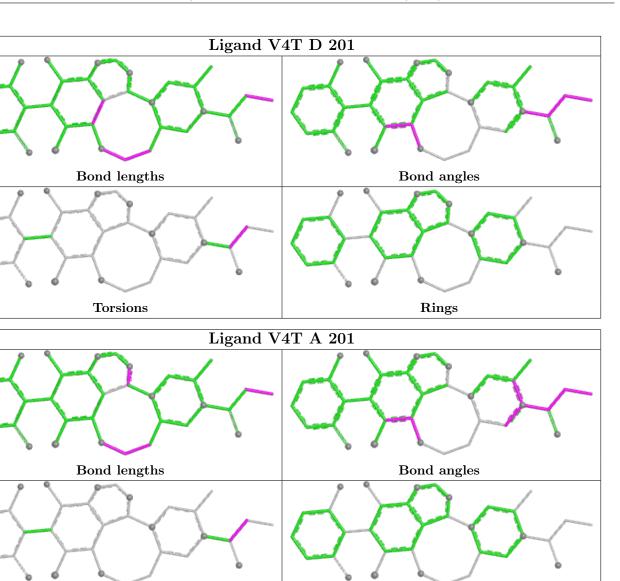
There are no ring outliers.

1 monomer is involved in 1 short contact:

[	Mol	Chain	Res	Type	Clashes	Symm-Clashes
	4	D	203	GDP	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 sufficient must be highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

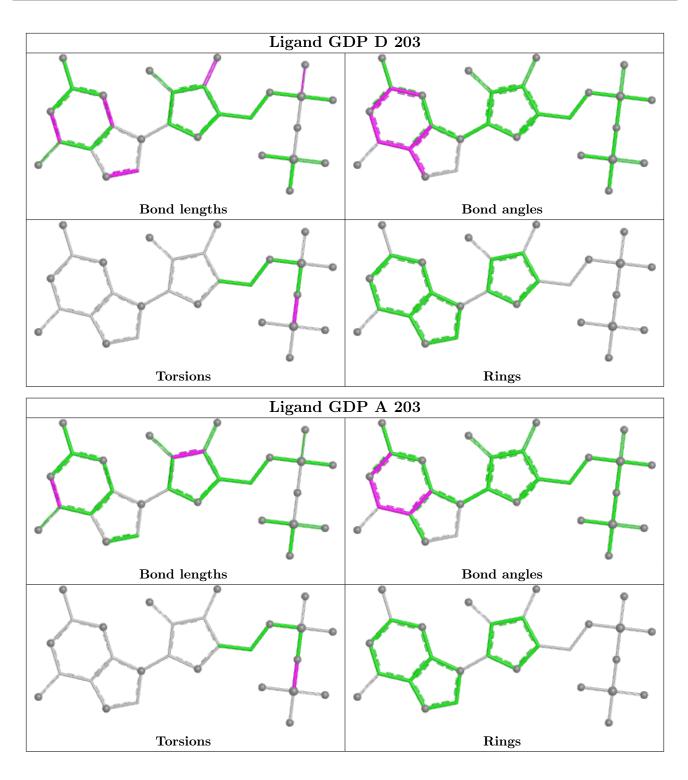




Rings



Torsions



### 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	$\langle RSRZ \rangle$	#RSRZ>2		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	168/170~(98%)	1.72	44 (26%) 0	1	7, 14, 27, 48	0
1	D	168/170~(98%)	1.68	45 (26%) 0	1	7, 13, 26, 40	0
All	All	336/340~(98%)	1.70	89 (26%) 0	1	7, 13, 27, 48	0

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	0	GLY	23.6
1	D	0	GLY	15.3
1	D	71	TYR	11.2
1	А	71	TYR	8.5
1	D	67	MET	7.5

### 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.

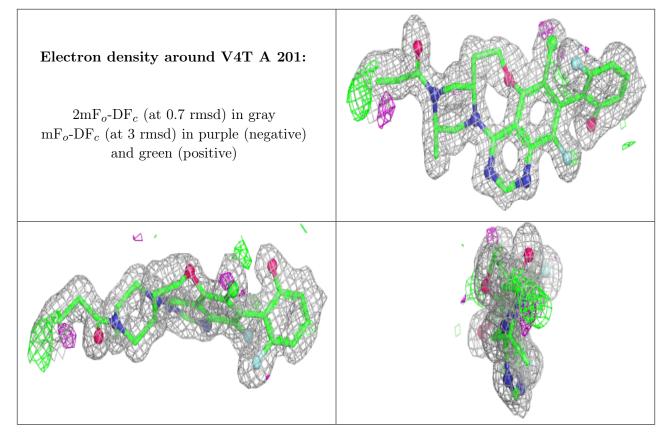
### 6.4 Ligands (i)

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.

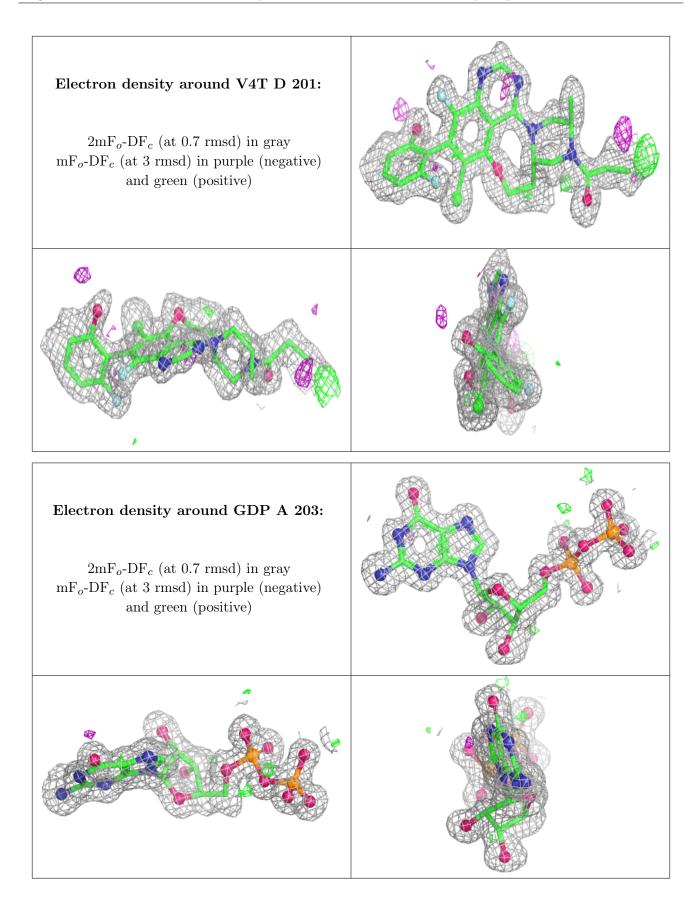


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	V4T	А	201	34/34	0.83	0.15	$15,\!18,\!22,\!26$	0
2	V4T	D	201	34/34	0.85	0.15	13,16,20,26	0
4	GDP	А	203	28/28	0.97	0.08	$10,\!11,\!15,\!17$	0
4	GDP	D	203	28/28	0.98	0.09	7,8,10,13	0
5	CA	D	204	1/1	0.98	0.11	$17,\!17,\!17,\!17$	0
3	MG	D	202	1/1	0.99	0.14	$6,\!6,\!6,\!6$	0
5	CA	А	204	1/1	0.99	0.07	11,11,11,11	0
3	MG	А	202	1/1	0.99	0.10	8,8,8,8	0

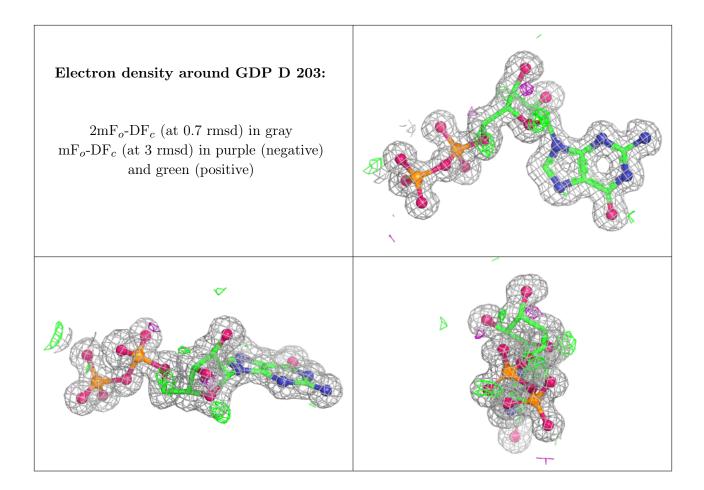
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.











### 6.5 Other polymers (i)

There are no such residues in this entry.

