



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2025 – 12:55 PM EDT

PDB ID : 9BG5  
Title : Tri-complex of Daraxonrasib (RMC-6236), KRAS G13D, and CypA  
Authors : Tomlinson, A.C.A.; Bieder, R.; Chen, A.; Knox, J.E.; Yano, J.K.  
Deposited on : 2024-04-18  
Resolution : 1.67 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

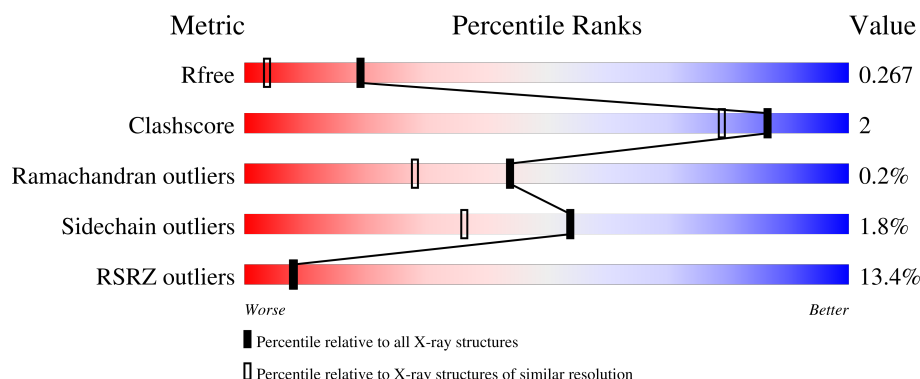
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 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))
$R_{free}$	164625	8422 (1.70-1.66)
Clashscore	180529	1005 (1.68-1.68)
Ramachandran outliers	177936	9065 (1.70-1.66)
Sidechain outliers	177891	9064 (1.70-1.66)
RSRZ outliers	164620	8421 (1.70-1.66)

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	170	<div> <div>5%</div> <div>95%</div> <div>5%</div> </div>
1	B	170	<div> <div>44%</div> <div>89%</div> <div>11%</div> </div>
2	C	166	<div> <div>2%</div> <div>96%</div> <div>2%</div> </div>
2	D	166	<div> <div>2%</div> <div>92%</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	A1AHB	C	201	X	-	-	-
5	A1AHB	D	201	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5980 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 GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	3	0
			1387	865	241	274	7			
1	B	170	Total	C	N	O	S	0	1	0
			1363	852	233	270	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P01116
A	13	ASP	GLY	engineered mutation	UNP P01116
A	151	GLY	ARG	conflict	UNP P01116
A	153	ASP	GLU	conflict	UNP P01116
A	165	LYS	-	expression tag	UNP P01116
A	166	HIS	-	expression tag	UNP P01116
A	167	LYS	-	expression tag	UNP P01116
A	168	GLU	-	expression tag	UNP P01116
A	169	LYS	-	expression tag	UNP P01116
B	0	SER	-	expression tag	UNP P01116
B	13	ASP	GLY	engineered mutation	UNP P01116
B	151	GLY	ARG	conflict	UNP P01116
B	153	ASP	GLU	conflict	UNP P01116
B	165	LYS	-	expression tag	UNP P01116
B	166	HIS	-	expression tag	UNP P01116
B	167	LYS	-	expression tag	UNP P01116
B	168	GLU	-	expression tag	UNP P01116
B	169	LYS	-	expression tag	UNP P01116

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	163	Total	C	N	O	S	0	0	0
			1248	792	216	232	8			

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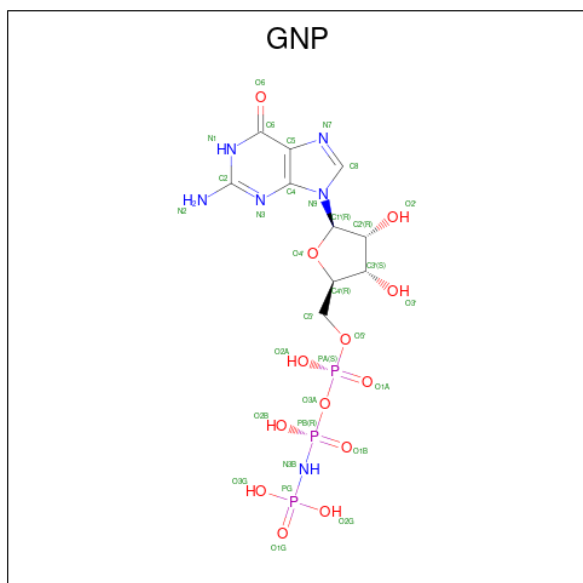
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	163	Total	C	N	O	S	0	1	0
			1252	795	216	233	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP P62937
D	0	SER	-	expression tag	UNP P62937

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).

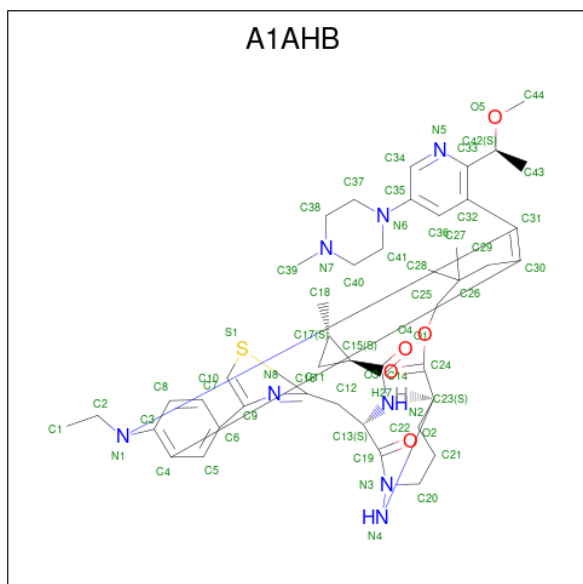


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is (1R,2S)-N-[(1P,7S,9S,13R,20M)-21-ethyl-20-{2-[(1R)-1-methoxyethyl]-5-(4-methylpiperazin-1-yl)pyridin-3-yl}-17,17-dimethyl-8,14-dioxo-15-oxa-4-thia-9,21,27,28-tetraazapentacyclo[17.5.2.1 2,5 .1 9,13 .0 22,26 ]octacos-1(24),2,5(28),19,22,25-hexaen-7-yl]-2-methylcyclopropane-1-carboxamide (three-letter code: A1AHB) (formula: C<sub>44</sub>H<sub>58</sub>N<sub>8</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	S	0	0
			58	44	8	5	1		
5	D	1	Total	C	N	O	S	0	0
			58	44	8	5	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	153	Total	O	0	3
			156	156		
6	B	88	Total	O	0	2
			90	90		
6	C	123	Total	O	0	2
			125	125		
6	D	175	Total	O	0	2
			177	177		

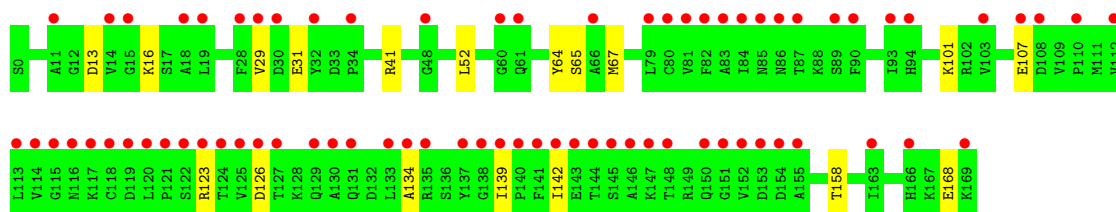
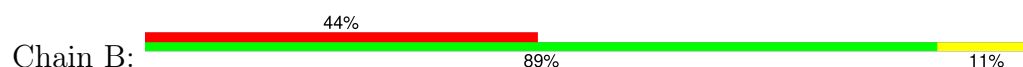
### 3 Residue-property plots [i](#)

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



- Molecule 1: GTPase KRas



- Molecule 2: Peptidyl-prolyl cis-trans isomerase A



- Molecule 2: Peptidyl-prolyl cis-trans isomerase A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.28Å 84.53Å 128.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.47 – 1.67 40.47 – 1.67	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.47-1.67) 99.9 (40.47-1.67)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 1.67Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.223 , 0.266 0.223 , 0.267	Depositor DCC
$R_{free}$ test set	4216 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5980	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1AHB, MG, GNP

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	0.37	0/1411	0.60	0/1901
1	B	0.30	0/1387	0.55	0/1870
2	C	0.37	0/1276	0.57	0/1711
2	D	0.43	0/1283	0.59	0/1721
All	All	0.37	0/5357	0.58	0/7203

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1387	0	1366	5	0
1	B	1363	0	1343	9	0
2	C	1248	0	1219	1	0
2	D	1252	0	1226	6	0
3	A	32	0	13	1	0
3	B	32	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	C	58	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	58	0	0	0	0
6	A	156	0	0	2	0
6	B	90	0	0	1	0
6	C	125	0	0	1	0
6	D	177	0	0	1	0
All	All	5980	0	5180	21	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 (21) 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)
2:D:81:GLU:HG2	2:D:82:LYS:HG3	1.81	0.61
1:A:41[B]:ARG:NH2	6:A:302:HOH:O	2.37	0.57
1:B:101:LYS:HD2	1:B:107:GLU:HG2	1.86	0.56
2:D:69:ARG:HG3	2:D:74:GLY:HA3	1.88	0.56
1:A:41[B]:ARG:NH1	1:A:52:LEU:HD21	2.23	0.54
1:B:65:SER:N	6:B:307:HOH:O	2.44	0.50
1:B:142:ILE:HD11	1:B:158:THR:HG21	1.92	0.50
2:D:84:GLU:H	2:D:84:GLU:CD	2.16	0.49
1:B:41:ARG:NH1	1:B:52:LEU:HD21	2.27	0.49
1:B:29:VAL:HG12	1:B:31:GLU:HB2	1.97	0.46
2:D:20:VAL:HG22	2:D:138:ILE:HB	1.97	0.46
1:B:134:ALA:HB1	1:B:139:ILE:O	2.17	0.45
2:D:82:LYS:HA	2:D:108:ASN:O	2.18	0.42
1:A:30:ASP:HA	3:A:201:GNP:O2'	2.19	0.42
1:B:64:TYR:HB3	1:B:67:MET:HG2	2.01	0.42
2:C:69:ARG:NH2	6:C:305:HOH:O	2.51	0.42
1:A:161:ARG:HD2	6:A:366:HOH:O	2.19	0.42
1:B:16:LYS:HB2	1:B:16:LYS:HE2	1.83	0.42
1:B:126:ASP:N	1:B:126:ASP:OD1	2.53	0.41
2:D:15:GLU:HG3	6:D:454:HOH:O	2.21	0.41
1:A:22:GLN:HG3	1:A:146:ALA:O	2.21	0.41

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	171/170 (101%)	164 (96%)	7 (4%)	0	100	100
1	B	169/170 (99%)	161 (95%)	7 (4%)	1 (1%)	22	9
2	C	161/166 (97%)	156 (97%)	5 (3%)	0	100	100
2	D	162/166 (98%)	159 (98%)	3 (2%)	0	100	100
All	All	663/672 (99%)	640 (96%)	22 (3%)	1 (0%)	44	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	123	ARG

### 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	154/151 (102%)	149 (97%)	5 (3%)	34	15
1	B	152/151 (101%)	150 (99%)	2 (1%)	65	50
2	C	131/134 (98%)	129 (98%)	2 (2%)	60	44
2	D	132/134 (98%)	130 (98%)	2 (2%)	60	44
All	All	569/570 (100%)	558 (98%)	11 (2%)	54	34

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	41[A]	ARG
1	A	41[B]	ARG
1	A	71	TYR
1	A	126	ASP
1	B	13	ASP
1	B	168	GLU
2	C	29	VAL
2	C	61	MET
2	D	29	VAL
2	D	61	MET

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	A1AHB	D	201	-	56,65,65	0.86	2 (3%)	64,97,97	1.01	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GNP	B	201	4	29,34,34	1.68	7 (24%)	33,54,54	2.25	6 (18%)
5	A1AHB	C	201	-	56,65,65	0.81	2 (3%)	64,97,97	1.08	3 (4%)
3	GNP	A	201	4	29,34,34	1.85	6 (20%)	33,54,54	2.18	6 (18%)

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
5	A1AHB	D	201	-	1/1/12/14	4/51/80/80	0/6/8/8
3	GNP	B	201	4	-	3/14/38/38	0/3/3/3
3	GNP	A	201	4	-	4/14/38/38	0/3/3/3
5	A1AHB	C	201	-	1/1/12/14	4/51/80/80	0/6/8/8

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	GNP	PB-O3A	5.50	1.65	1.59
5	D	201	A1AHB	C29-C26	-4.12	1.54	1.55
3	B	201	GNP	PB-O3A	3.88	1.63	1.59
3	A	201	GNP	PB-O1B	3.86	1.52	1.46
3	B	201	GNP	PB-O1B	3.83	1.52	1.46
3	B	201	GNP	PG-N3B	3.64	1.72	1.63
3	A	201	GNP	C6-N1	3.50	1.39	1.33
3	A	201	GNP	PG-N3B	3.27	1.71	1.63
3	B	201	GNP	C6-N1	3.11	1.38	1.33
3	A	201	GNP	PB-O2B	-2.96	1.48	1.56
3	A	201	GNP	PG-O1G	2.85	1.50	1.46
3	B	201	GNP	PG-O1G	2.83	1.50	1.46
5	C	201	A1AHB	C19-N3	2.63	1.39	1.35
5	C	201	A1AHB	C15-C14	-2.63	1.47	1.51
3	B	201	GNP	PB-O2B	-2.47	1.50	1.56
5	D	201	A1AHB	C15-C14	-2.23	1.48	1.51
3	B	201	GNP	C5-C6	2.12	1.45	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	GNP	C5-C6-N1	-8.50	112.05	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	GNP	C5-C6-N1	-8.46	112.10	123.42
3	B	201	GNP	C2-N1-C6	6.67	125.23	115.96
3	A	201	GNP	C2-N1-C6	6.50	124.99	115.96
5	C	201	A1AHB	C41-N6-C37	3.75	120.00	111.57
3	B	201	GNP	O1G-PG-N3B	-3.51	106.61	111.77
3	B	201	GNP	N3-C2-N1	-2.96	123.45	127.21
3	A	201	GNP	N3-C2-N1	-2.74	123.72	127.21
5	C	201	A1AHB	C32-C31-C30	-2.56	125.31	129.40
3	A	201	GNP	O2G-PG-O1G	-2.45	107.31	113.45
3	A	201	GNP	O2G-PG-O3G	2.42	114.08	107.59
3	B	201	GNP	C2-N3-C4	-2.41	112.89	115.48
3	A	201	GNP	C2-N3-C4	-2.34	112.96	115.48
3	B	201	GNP	O1B-PB-N3B	-2.28	108.41	111.77
5	D	201	A1AHB	C41-N6-C37	2.17	116.46	111.57
5	D	201	A1AHB	C2-N1-C31	2.08	128.04	124.36
5	C	201	A1AHB	C38-C37-N6	2.06	115.12	110.78
5	D	201	A1AHB	O4-C25-C26	-2.00	105.81	109.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	201	A1AHB	N3
5	D	201	A1AHB	N3

All (15) torsion outliers are listed below:

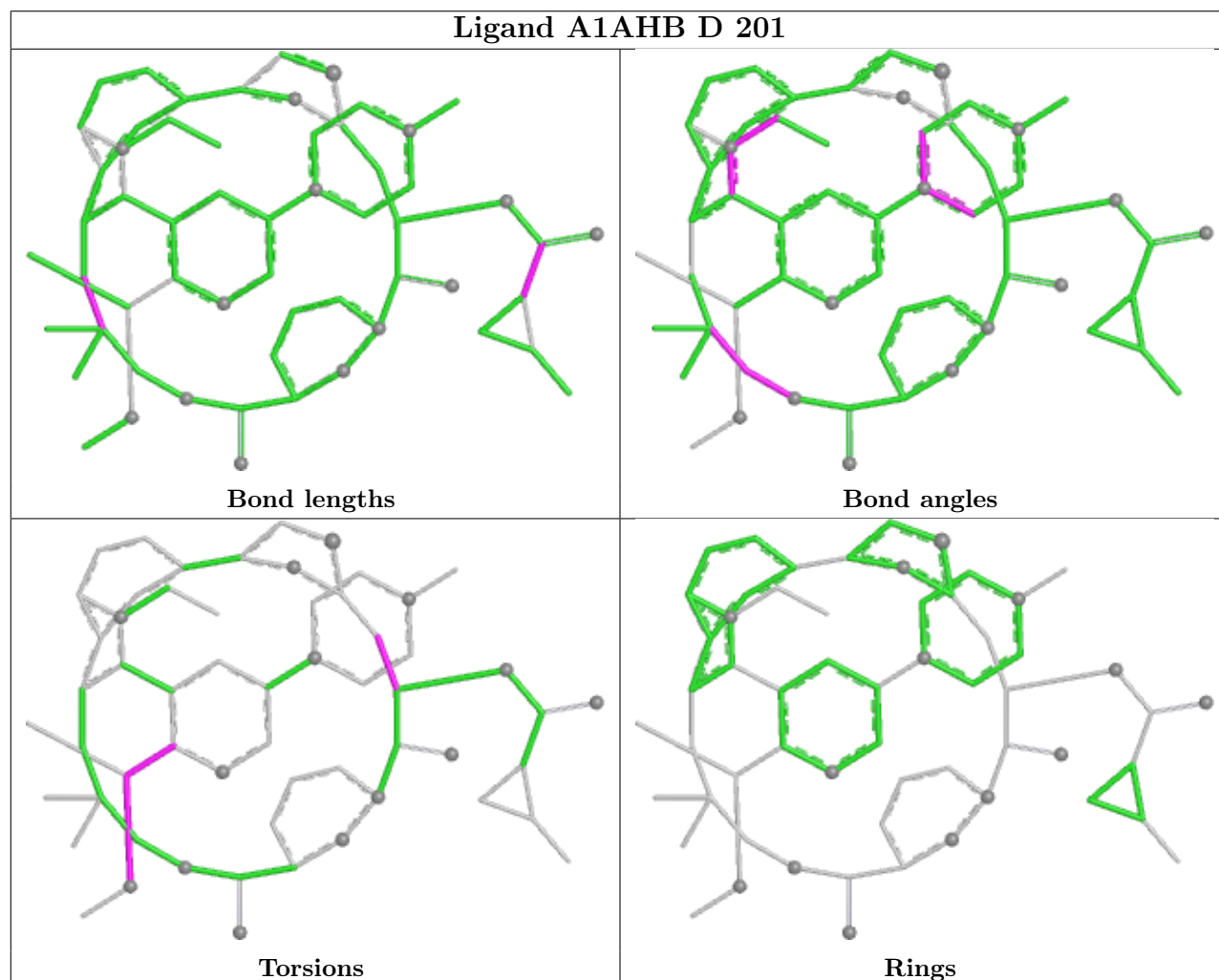
Mol	Chain	Res	Type	Atoms
3	A	201	GNP	PB-N3B-PG-O1G
3	A	201	GNP	PG-N3B-PB-O1B
3	A	201	GNP	PA-O3A-PB-O2B
3	B	201	GNP	PB-N3B-PG-O1G
3	B	201	GNP	PG-N3B-PB-O1B
5	C	201	A1AHB	C32-C33-C42-C43
5	D	201	A1AHB	C32-C33-C42-C43
5	C	201	A1AHB	C11-C12-C13-C19
5	D	201	A1AHB	C11-C12-C13-C19
5	C	201	A1AHB	C32-C33-C42-O5
5	D	201	A1AHB	C32-C33-C42-O5
5	D	201	A1AHB	C33-C42-O5-C44
5	C	201	A1AHB	C33-C42-O5-C44
3	A	201	GNP	PA-O3A-PB-O1B
3	B	201	GNP	PG-N3B-PB-O3A

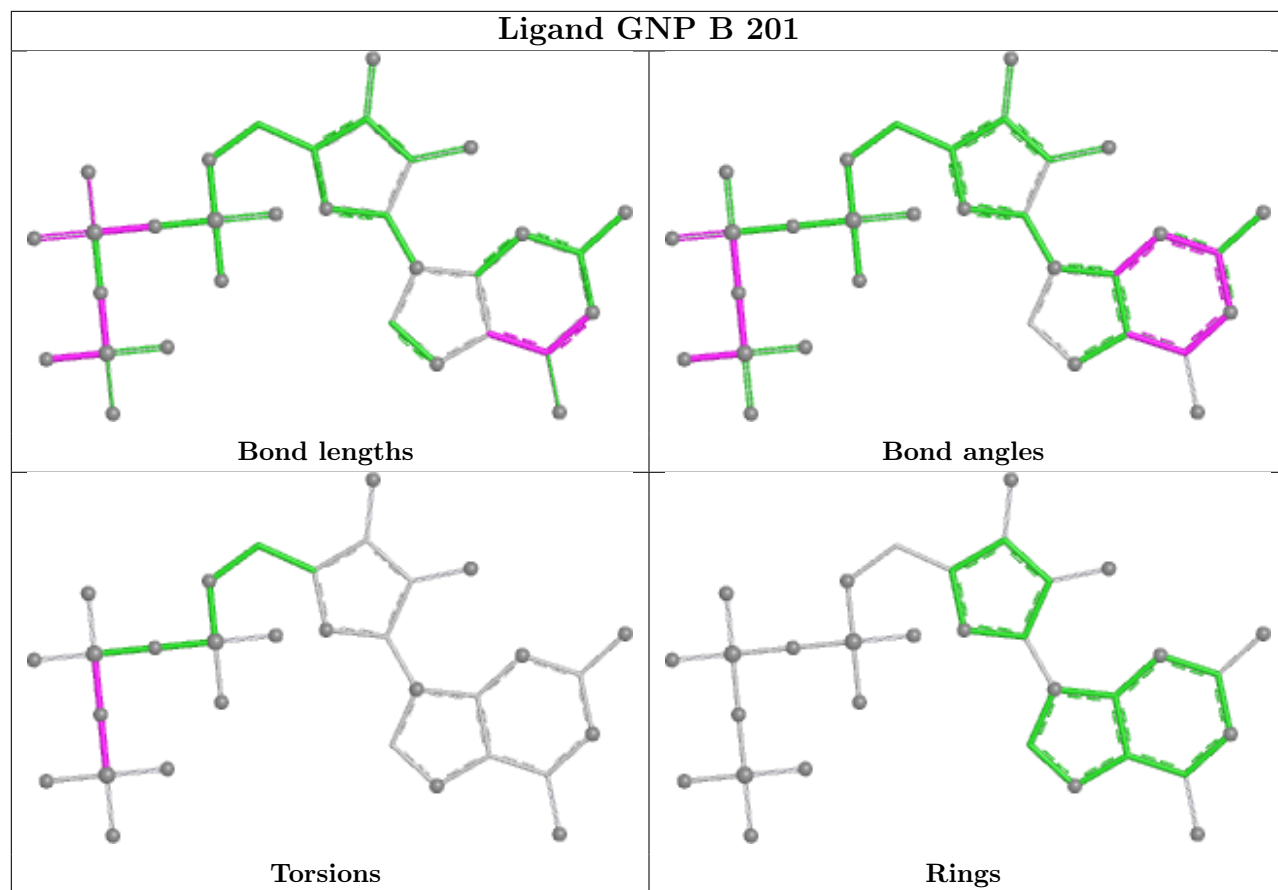
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	GNP	1	0

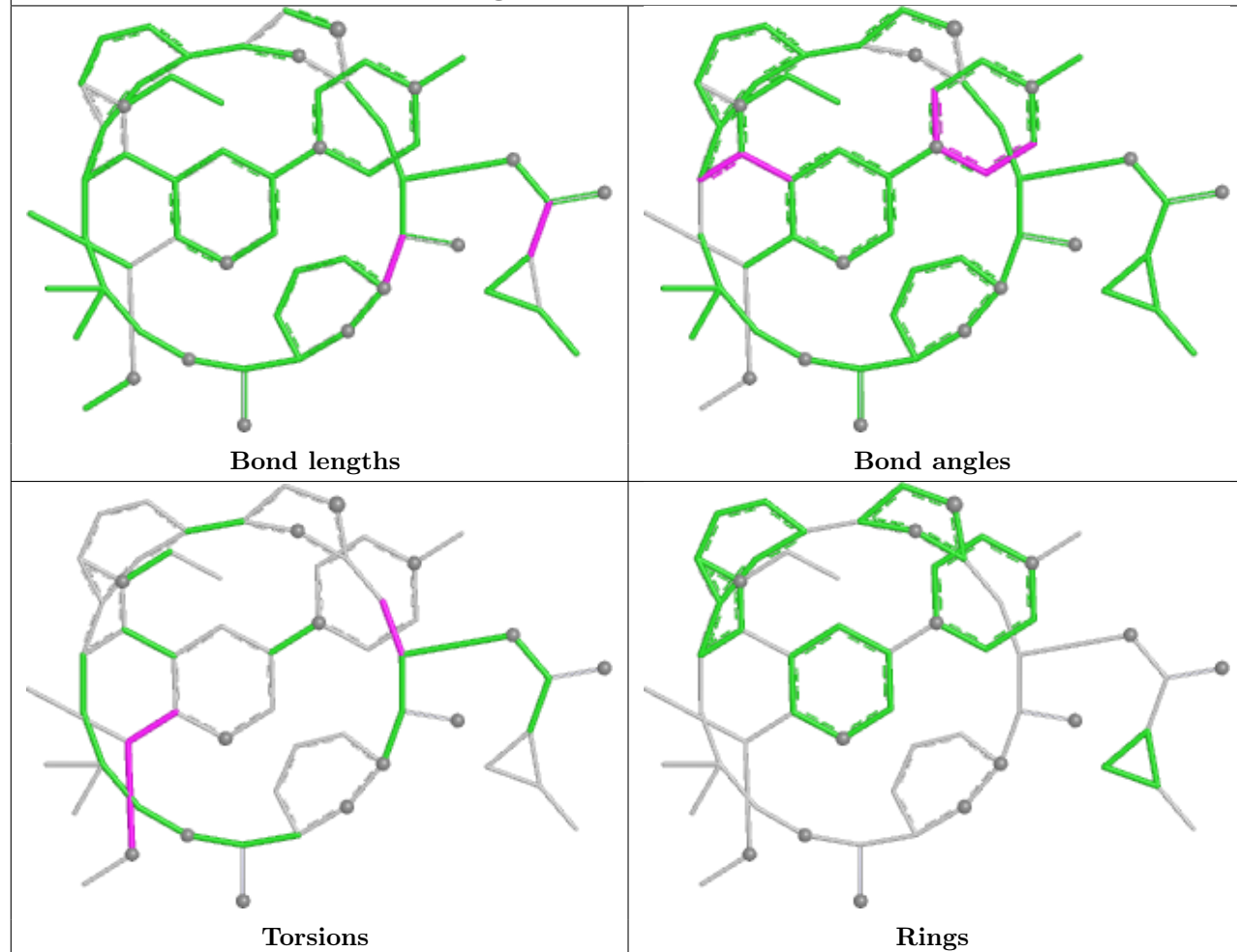
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

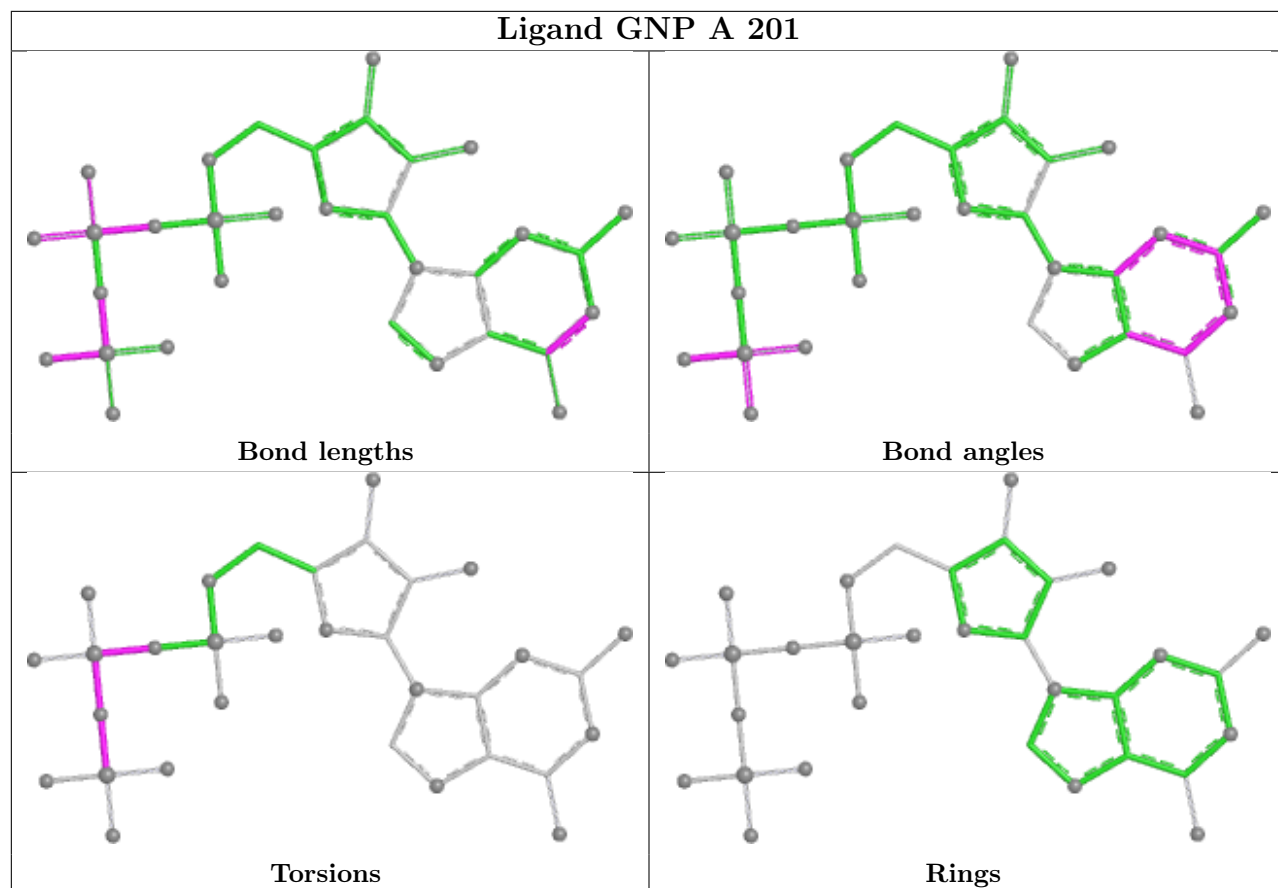






## Ligand A1AHB C 201





## 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	170/170 (100%)	0.40	9 (5%) 33 36	14, 33, 56, 93	3 (1%)
1	B	170/170 (100%)	1.89	74 (43%) 1 0	25, 52, 96, 110	1 (0%)
2	C	163/166 (98%)	0.47	3 (1%) 67 71	23, 34, 49, 60	0
2	D	163/166 (98%)	0.12	3 (1%) 67 71	20, 28, 41, 53	1 (0%)
All	All	666/672 (99%)	0.73	89 (13%) 8 8	14, 35, 72, 110	5 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	LEU	6.3
1	B	118[A]	CYS	5.7
1	B	121	PRO	5.1
1	B	84	ILE	5.0
1	B	127	THR	4.9
1	B	83	ALA	4.9
1	B	125	VAL	4.7
1	A	32	TYR	4.5
1	B	82	PHE	4.5
1	B	139	ILE	4.4
1	B	142	ILE	4.4
1	B	113	LEU	4.4
1	B	130	ALA	4.2
1	B	29	VAL	4.2
1	B	28	PHE	4.1
1	B	141	PHE	4.1
1	B	148	THR	4.1
1	B	144	THR	4.0
1	B	90	PHE	3.9
2	C	2	VAL	3.9
1	B	147	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	124	THR	3.7
1	B	114	VAL	3.6
1	B	123	ARG	3.6
1	B	115	GLY	3.6
1	A	0	SER	3.5
1	B	79	LEU	3.4
1	B	152	VAL	3.4
1	B	122	SER	3.3
1	B	146	ALA	3.3
1	B	134	ALA	3.2
1	B	116	ASN	3.2
1	B	32	TYR	3.2
1	B	143	GLU	3.1
1	B	112	VAL	3.1
1	B	140	PRO	3.1
2	D	2	VAL	3.1
1	B	93	ILE	3.1
1	B	87	THR	3.0
1	B	19	LEU	3.0
1	B	133	LEU	3.0
1	B	119	ASP	2.8
1	B	94	HIS	2.8
1	B	81	VAL	2.7
1	B	166	HIS	2.7
1	B	15	GLY	2.7
1	B	89	SER	2.6
1	B	110	PRO	2.6
1	B	107	GLU	2.6
1	B	61	GLN	2.6
1	B	150	GLN	2.6
1	B	103	VAL	2.6
1	B	126	ASP	2.5
1	B	153	ASP	2.5
1	B	60	GLY	2.5
1	A	121	PRO	2.5
1	B	154	ASP	2.5
1	B	138	GLY	2.5
2	D	164	LEU	2.5
1	B	155	ALA	2.5
1	B	85	ASN	2.4
1	B	48	GLY	2.4
1	B	34	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	145	SER	2.4
1	B	137	TYR	2.4
1	B	169	LYS	2.3
2	C	164	LEU	2.3
1	B	117	LYS	2.3
1	B	30	ASP	2.3
2	D	5[A]	THR	2.3
1	B	66	ALA	2.2
1	B	135	ARG	2.2
1	B	86	ASN	2.2
1	B	129	GLN	2.2
1	A	94	HIS	2.2
1	B	18	ALA	2.1
1	B	163	ILE	2.1
1	B	80	CYS	2.1
1	B	108	ASP	2.1
1	B	11	ALA	2.1
1	A	62	GLU	2.1
1	B	151	GLY	2.1
2	C	50	GLY	2.1
1	A	103	VAL	2.1
1	A	168	GLU	2.0
1	B	131	GLN	2.0
1	B	14	VAL	2.0
1	A	127	THR	2.0
1	A	108	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

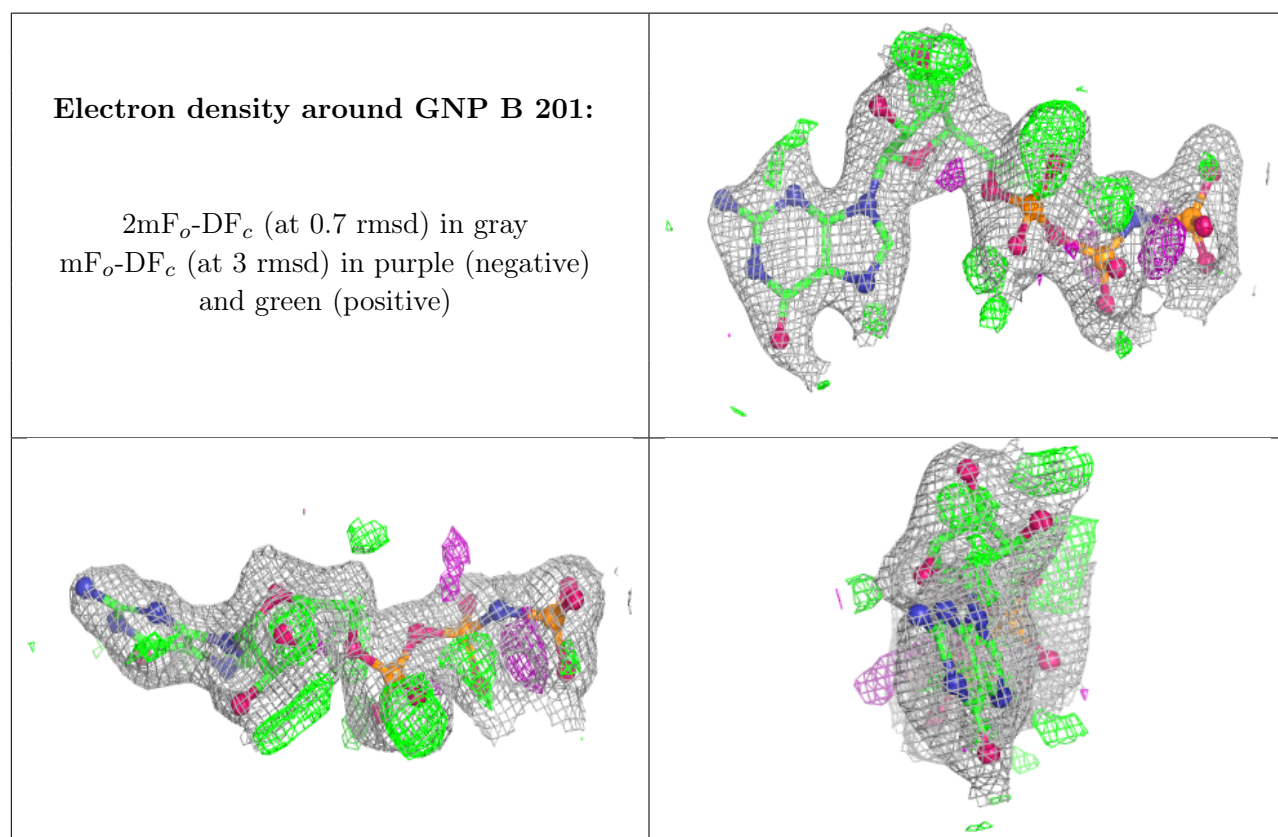
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

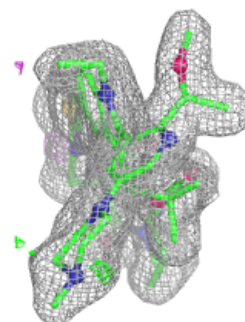
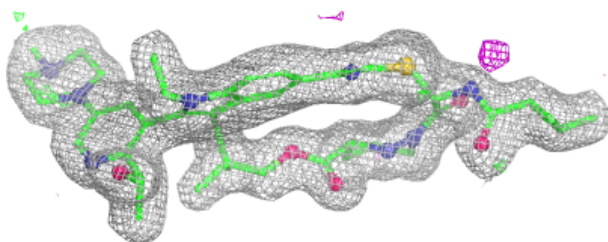
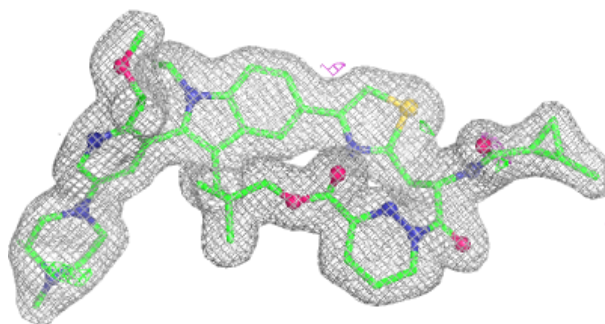
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GNP	B	201	32/32	0.91	0.12	33,50,59,63	0
4	MG	B	202	1/1	0.95	0.06	32,32,32,32	0
5	A1AHB	C	201	58/58	0.96	0.07	20,25,37,39	0
5	A1AHB	D	201	58/58	0.97	0.06	17,21,28,37	0
3	GNP	A	201	32/32	0.98	0.05	19,25,31,37	0
4	MG	A	202	1/1	0.99	0.02	23,23,23,23	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.

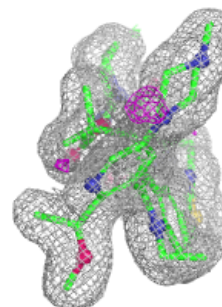
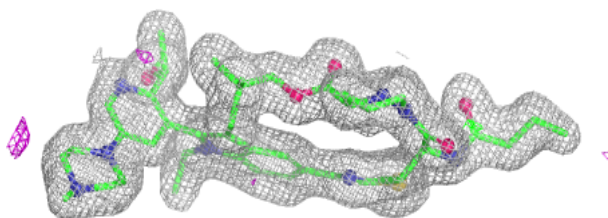
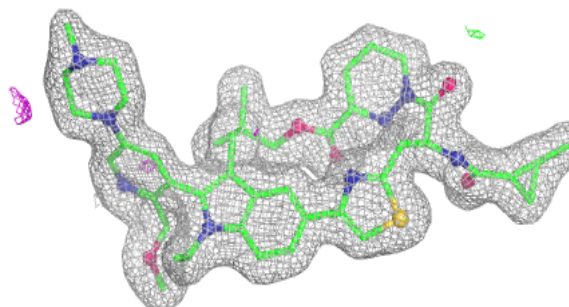


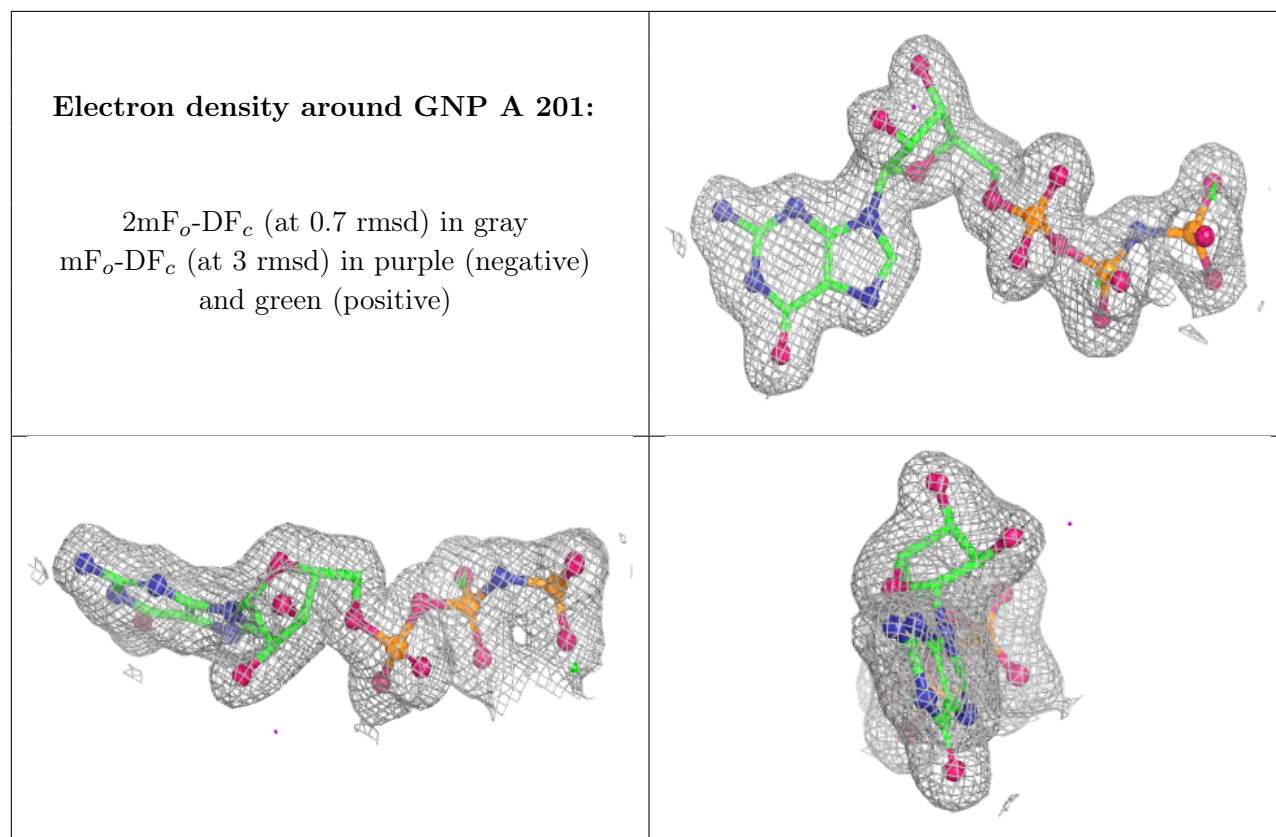
**Electron density around A1AHB C 201:**

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

**Electron density around A1AHB D 201:**

$2mF_o-DF_c$  (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.