



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:08 am BST

PDB ID : 6D55  
Title : Ras:SOS:Ras in complex with a small molecule activator  
Authors : Phan, J.; Hodges, T.; Fesik, S.W.  
Deposited on : 2018-04-19  
Resolution : 1.68 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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

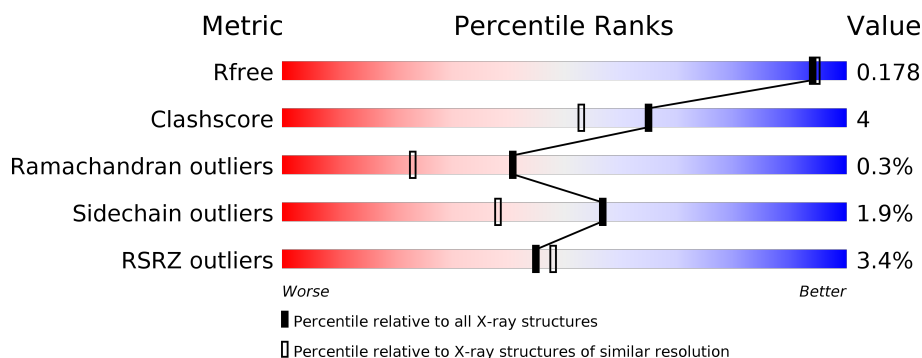
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.68 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (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 on 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	167	<div> <div>2%</div> <div>92%</div> <div>7%</div> <div>..</div> </div>
2	B	482	<div> <div>2%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
3	C	167	<div> <div>10%</div> <div>84%</div> <div>13%</div> <div>.</div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8143 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 HRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	9	0
			1392	861	242	281	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P01112
A	64	ALA	TYR	conflict	UNP P01112

- Molecule 2 is a protein called Son of sevenless homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	469	Total	C	N	O	S	0	23	0
			4097	2612	709	763	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	565	GLY	-	expression tag	UNP Q07889

- Molecule 3 is a protein called GTPase HRas.

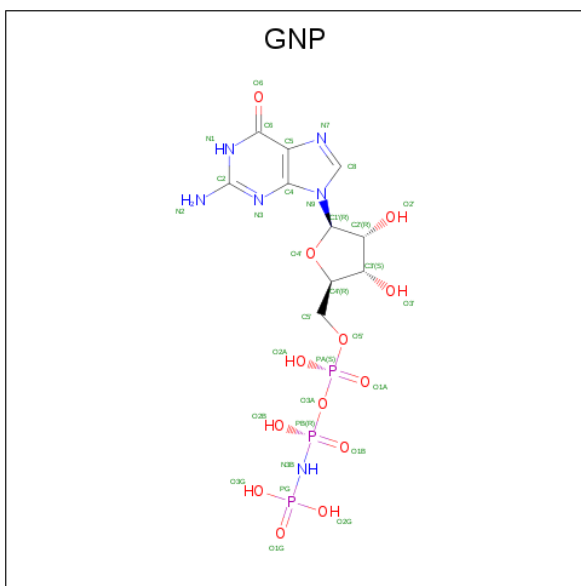
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	167	Total	C	N	O	S	0	8	0
			1391	865	240	279	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP P01112

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter

code: GNP) (formula:  $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{13}\text{P}_3$ ).

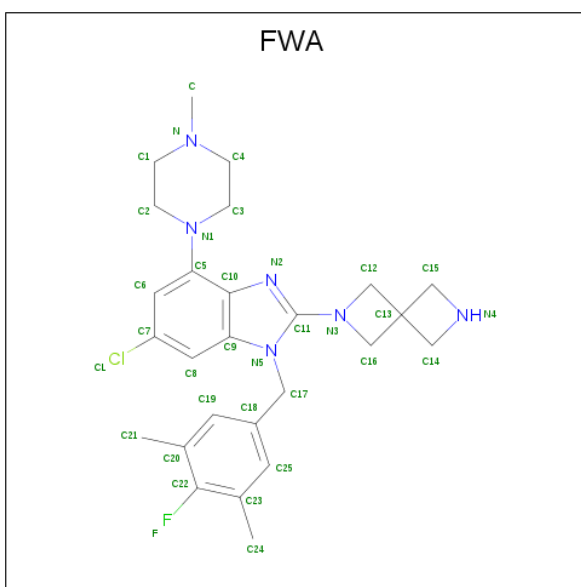


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

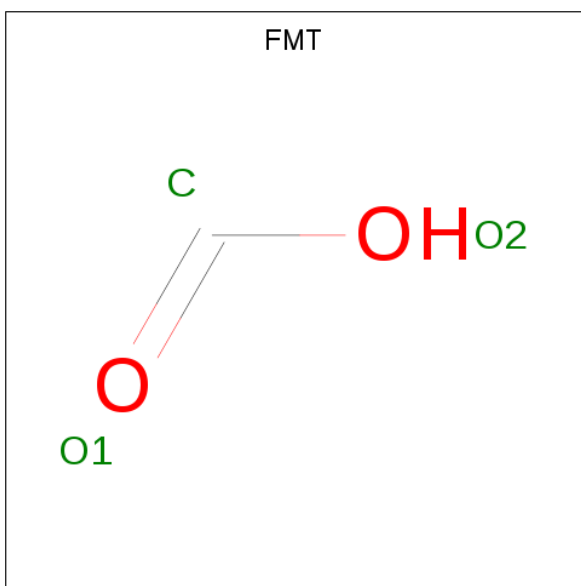
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

- Molecule 6 is 6-chloro-2-(2,6-diazaspiro[3.3]heptan-2-yl)-1-[(4-fluoro-3,5-dimethylphenyl)methyl]-4-(4-methylpiperazin-1-yl)-1H-benzimidazole (three-letter code: FWA) (formula:  $\text{C}_{26}\text{H}_{32}\text{ClFN}_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Cl	F	N	0	0
			34	26	1	1	6		

- Molecule 7 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			3	1	2		
7	B	1	Total	C	O	0	0
			3	1	2		
7	B	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			3	1	2		
7	B	1	Total	C	O	0	0
			3	1	2		
7	C	1	Total	C	O	0	0
			3	1	2		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	Na	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	188	Total	O	0	0
			188	188		

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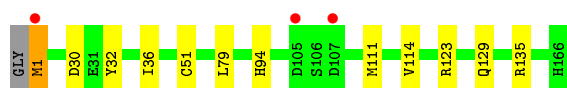
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	754	Total 754	O 754	0	0
10	C	223	Total 223	O 223	0	0

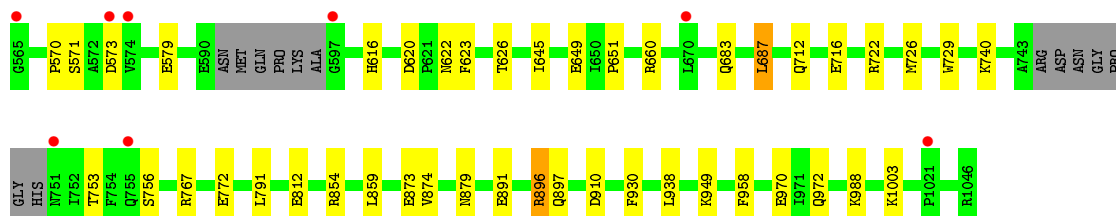
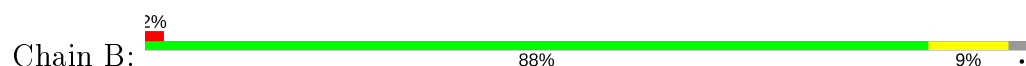
### 3 Residue-property plots [i](#)

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.

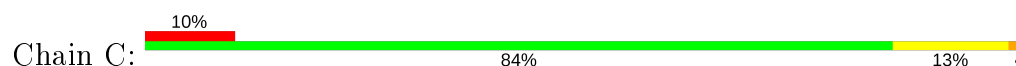
- Molecule 1: GTPase HRas



- Molecule 2: Son of sevenless homolog 1



- Molecule 3: GTPase HRas





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.48Å 183.48Å 179.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.03 – 1.68 41.03 – 1.68	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.03-1.68) 99.9 (41.03-1.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 1.68Å)	Xtriage
Refinement program	PHENIX (dev_2875: ???)	Depositor
R, $R_{free}$	0.156 , 0.178 0.156 , 0.178	Depositor DCC
$R_{free}$ test set	1987 reflections (1.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for l,-k,h 0.006 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CSO, NA, FMT, MG, GNP, FWA

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	0.73	0/1402	0.82	3/1888 (0.2%)
2	B	0.78	3/4190 (0.1%)	0.87	8/5661 (0.1%)
3	C	0.77	0/1410	0.80	0/1901
All	All	0.77	3/7002 (0.0%)	0.85	11/9450 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	873	GLU	CD-OE1	6.35	1.32	1.25
2	B	873	GLU	CD-OE2	-6.23	1.18	1.25
2	B	873	GLU	CB-CG	-5.70	1.41	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	660[A]	ARG	NE-CZ-NH1	11.78	126.19	120.30
2	B	660[B]	ARG	NE-CZ-NH1	11.78	126.19	120.30
2	B	660[A]	ARG	NE-CZ-NH2	-8.35	116.12	120.30
2	B	660[B]	ARG	NE-CZ-NH2	-8.35	116.12	120.30
2	B	767	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	123	ARG	NE-CZ-NH1	6.68	123.64	120.30
2	B	854	ARG	NE-CZ-NH2	-6.07	117.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ARG	NE-CZ-NH2	-5.79	117.40	120.30
2	B	767	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	135	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	B	722	ARG	C-N-CA	-5.17	111.45	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	25	GLN	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1392	0	1352	7	0
2	B	4097	0	4079	30	0
3	C	1391	0	1358	20	0
4	A	32	0	13	0	0
5	A	1	0	0	0	0
6	B	34	0	0	0	0
7	B	15	0	5	1	0
7	C	3	0	1	1	0
8	B	12	0	15	0	0
9	C	1	0	0	0	0
10	A	188	0	0	3	0
10	B	754	0	0	17	1
10	C	223	0	0	8	1
All	All	8143	0	6823	57	1

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 4.

All (57) 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)
3:C:117[A]:LYS:NZ	10:C:301:HOH:O	2.00	0.94
2:B:891[B]:GLU:OE1	10:B:2101:HOH:O	1.93	0.85
2:B:891[A]:GLU:HG2	10:B:2153:HOH:O	1.78	0.82
2:B:988[B]:LYS:NZ	10:B:2103:HOH:O	2.13	0.79
3:C:39:SER:HA	10:C:303:HOH:O	1.86	0.75
1:A:94:HIS:ND1	10:A:302:HOH:O	2.19	0.75
1:A:129:GLN:OE1	10:A:301:HOH:O	2.10	0.69
7:C:201:FMT:O2	10:C:302:HOH:O	2.11	0.69
2:B:772:GLU:OE2	10:B:2104:HOH:O	2.13	0.66
2:B:812:GLU:OE1	10:B:2106:HOH:O	2.14	0.66
2:B:620:ASP:OD1	10:B:2105:HOH:O	2.13	0.64
2:B:616:HIS:ND1	7:B:2005:FMT:O2	2.31	0.63
2:B:579:GLU:HB3	10:B:2251:HOH:O	2.01	0.61
3:C:85:ASN:HD22	3:C:121:ALA:HB3	1.69	0.58
2:B:623:PHE:HE1	2:B:958:PHE:CE2	2.25	0.55
2:B:859[B]:LEU:HD23	2:B:874:VAL:HB	1.88	0.55
2:B:910[A]:ASP:OD1	10:B:2107:HOH:O	2.19	0.54
3:C:99[B]:GLN:O	3:C:103[B]:VAL:HG23	2.10	0.52
1:A:36:ILE:HG23	2:B:687:LEU:HD13	1.90	0.52
3:C:119:ASP:HB2	10:C:412:HOH:O	2.09	0.51
3:C:24:ILE:HD13	3:C:42:LYS:HB2	1.93	0.51
2:B:712:GLN:O	2:B:716[B]:GLU:HG2	2.12	0.50
2:B:687:LEU:HD23	2:B:726:MET:SD	2.52	0.49
3:C:41:ARG:NH1	3:C:54:ASP:OD2	2.45	0.49
2:B:622[B]:ASN:O	2:B:626[B]:THR:HG23	2.12	0.49
2:B:570:PRO:HB3	2:B:651:PRO:HG2	1.93	0.49
3:C:29:VAL:HG12	3:C:31:GLU:HB2	1.95	0.49
3:C:38:ASP:OD1	3:C:38:ASP:N	2.45	0.48
3:C:40:TYR:HB3	10:C:377:HOH:O	2.14	0.48
3:C:36:ILE:HG13	3:C:36:ILE:O	2.14	0.47
2:B:972[B]:GLN:HG2	10:B:2269:HOH:O	2.15	0.47
2:B:571:SER:OG	2:B:573:ASP:OD1	2.25	0.46
2:B:972[A]:GLN:NE2	10:B:2109:HOH:O	2.27	0.46
2:B:791:LEU:HD12	10:B:2528:HOH:O	2.17	0.45
3:C:24:ILE:HG21	3:C:39:SER:O	2.17	0.45
1:A:1:MET:N	10:A:310:HOH:O	2.51	0.44
2:B:623:PHE:CE1	2:B:958:PHE:CE2	3.05	0.44
3:C:38:ASP:O	10:C:303:HOH:O	2.21	0.44
2:B:938[A]:LEU:HD12	10:B:2415:HOH:O	2.17	0.43
3:C:166:HIS:HD2	10:C:460:HOH:O	2.00	0.43
1:A:1:MET:HG2	1:A:51:CSO:HA	2.01	0.43
3:C:27:HIS:ND1	3:C:27:HIS:C	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:HIS:N	10:C:310:HOH:O	2.52	0.43
2:B:687:LEU:HD21	2:B:729:TRP:CE3	2.54	0.42
2:B:645:ILE:O	2:B:649[B]:GLU:HG2	2.19	0.42
2:B:1003:LYS:NZ	10:B:2135:HOH:O	2.52	0.42
3:C:27:HIS:CE1	3:C:149:ARG:HD3	2.54	0.42
3:C:27:HIS:C	3:C:27:HIS:HD1	2.23	0.42
3:C:19[A]:LEU:HD11	3:C:114:VAL:HG11	2.01	0.42
2:B:970[B]:GLU:HG3	10:B:2322:HOH:O	2.20	0.42
2:B:896[A]:ARG:HG3	2:B:897:GLN:N	2.35	0.41
2:B:891[A]:GLU:HG3	10:B:2101:HOH:O	2.21	0.41
1:A:79[B]:LEU:HG	1:A:114:VAL:HG21	2.02	0.41
2:B:683:GLN:HG2	10:B:2238:HOH:O	2.20	0.41
2:B:949:LYS:NZ	10:B:2134:HOH:O	2.51	0.41
3:C:127[B]:SER:O	3:C:131[B]:GLN:HG3	2.21	0.40
1:A:111[B]:MET:HB3	1:A:111[B]:MET:HE3	1.75	0.40

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)
10:B:2722:HOH:O	10:C:495:HOH:O[3_555]	2.11	0.09

## 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	Percentiles	
1	A	172/167 (103%)	170 (99%)	2 (1%)	0	100	100
2	B	488/482 (101%)	483 (99%)	5 (1%)	0	100	100
3	C	173/167 (104%)	166 (96%)	5 (3%)	2 (1%)	13	2
All	All	833/816 (102%)	819 (98%)	12 (1%)	2 (0%)	41	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	26	ASN
3	C	37	GLU

### 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	151/142 (106%)	148 (98%)	3 (2%)	55	36
2	B	462/447 (103%)	454 (98%)	8 (2%)	60	43
3	C	152/144 (106%)	147 (97%)	5 (3%)	38	16
All	All	765/733 (104%)	749 (98%)	16 (2%)	57	33

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	30	ASP
1	A	32	TYR
2	B	687	LEU
2	B	740	LYS
2	B	753	THR
2	B	756	SER
2	B	879	ASN
2	B	896[A]	ARG
2	B	896[B]	ARG
2	B	930	PHE
3	C	27	HIS
3	C	31	GLU
3	C	38	ASP
3	C	127[A]	SER
3	C	127[B]	SER

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

Mol	Chain	Res	Type
1	A	94	HIS
3	C	166	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z  > 2$
1	CSO	A	51	1	3,6,7	1.70	1 (33%)	0,6,8	0.00	-

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
1	CSO	A	51	1	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	CSO	CB-CA	-2.64	1.46	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	51	CSO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	FWA	B	2001	-	31,39,39	1.69	5 (16%)	33,60,60	2.67	12 (36%)
7	FMT	B	2002	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	2005	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	C	201	-	0,2,2	0.00	-	0,1,1	0.00	-
8	GOL	B	2007	-	5,5,5	1.26	1 (20%)	5,5,5	1.12	0
7	FMT	B	2003	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	2004	-	0,2,2	0.00	-	0,1,1	0.00	-
4	GNP	A	201	5	28,34,34	2.26	6 (21%)	30,54,54	1.79	3 (10%)
8	GOL	B	2008	-	5,5,5	1.28	0	5,5,5	1.02	1 (20%)
7	FMT	B	2006	-	0,2,2	0.00	-	0,1,1	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FWA	B	2001	-	-	2/8/40/40	0/6/6/6
4	GNP	A	201	5	-	5/17/38/38	0/3/3/3
8	GOL	B	2007	-	-	0/4/4/4	-
8	GOL	B	2008	-	-	2/4/4/4	-



All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	GNP	C4-N9	-6.96	1.38	1.47
4	A	201	GNP	C5-C6	-4.68	1.44	1.52
4	A	201	GNP	PG-O1G	4.55	1.53	1.46
6	B	2001	FWA	C15-C13	4.27	1.58	1.54
4	A	201	GNP	C6-N1	3.94	1.39	1.33
6	B	2001	FWA	C16-C13	3.36	1.57	1.54
6	B	2001	FWA	C19-C18	3.15	1.44	1.39
6	B	2001	FWA	C2-N1	2.82	1.51	1.46
8	B	2007	GOL	C3-C2	2.73	1.62	1.51
4	A	201	GNP	PB-N3B	2.69	1.70	1.63
6	B	2001	FWA	C7-CL	2.42	1.79	1.74
4	A	201	GNP	PB-O2B	-2.21	1.50	1.56

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2001	FWA	C25-C23-C22	6.79	121.07	116.21
6	B	2001	FWA	C8-C7-C6	6.66	129.97	121.66
4	A	201	GNP	C4-C5-N7	5.73	110.05	102.46
6	B	2001	FWA	C8-C7-CL	-4.92	113.49	119.64
6	B	2001	FWA	C19-C20-C22	4.76	119.62	116.21
4	A	201	GNP	C5-C6-N1	-4.76	112.32	118.19
6	B	2001	FWA	C7-C8-C9	-4.50	111.31	118.62
4	A	201	GNP	O6-C6-C5	3.76	127.53	119.86
6	B	2001	FWA	C16-C13-C12	3.70	91.46	85.68
6	B	2001	FWA	C6-C5-C10	-3.23	115.02	120.12
6	B	2001	FWA	C20-C19-C18	-3.00	118.75	122.21
6	B	2001	FWA	C23-C25-C18	-2.72	119.06	122.21
6	B	2001	FWA	C8-C9-C10	2.50	122.92	120.55
8	B	2008	GOL	C3-C2-C1	-2.14	103.40	111.70
6	B	2001	FWA	C6-C7-CL	-2.11	116.52	119.15
6	B	2001	FWA	C9-C10-N2	2.05	112.38	107.99

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	201	GNP	PB-N3B-PG-O1G
4	A	201	GNP	PG-N3B-PB-O1B
4	A	201	GNP	C2'-C1'-N9-C4
8	B	2008	GOL	C1-C2-C3-O3

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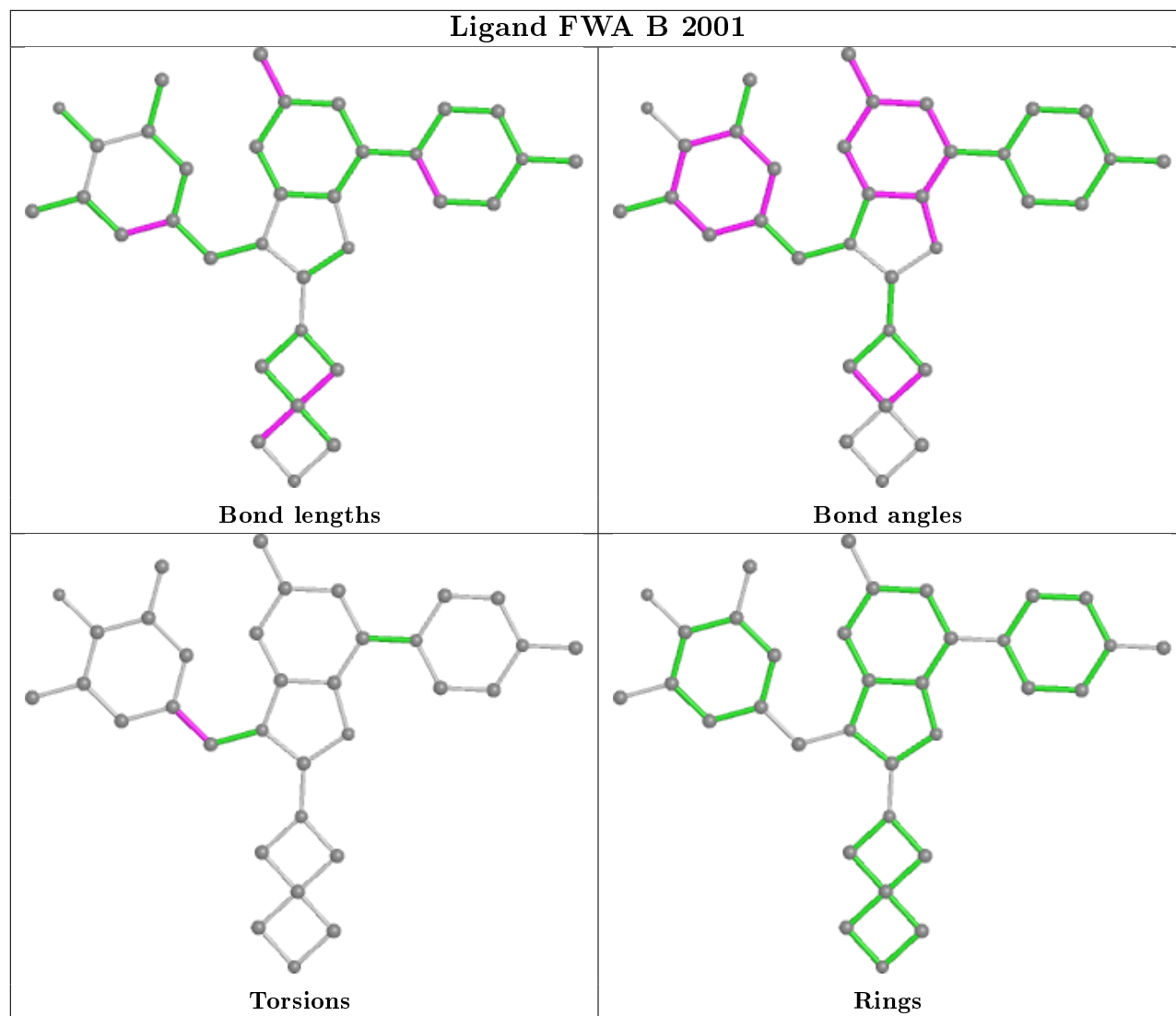
Mol	Chain	Res	Type	Atoms
8	B	2008	GOL	O2-C2-C3-O3
6	B	2001	FWA	N5-C17-C18-C25
6	B	2001	FWA	N5-C17-C18-C19
4	A	201	GNP	PA-O3A-PB-O2B
4	A	201	GNP	PG-N3B-PB-O3A

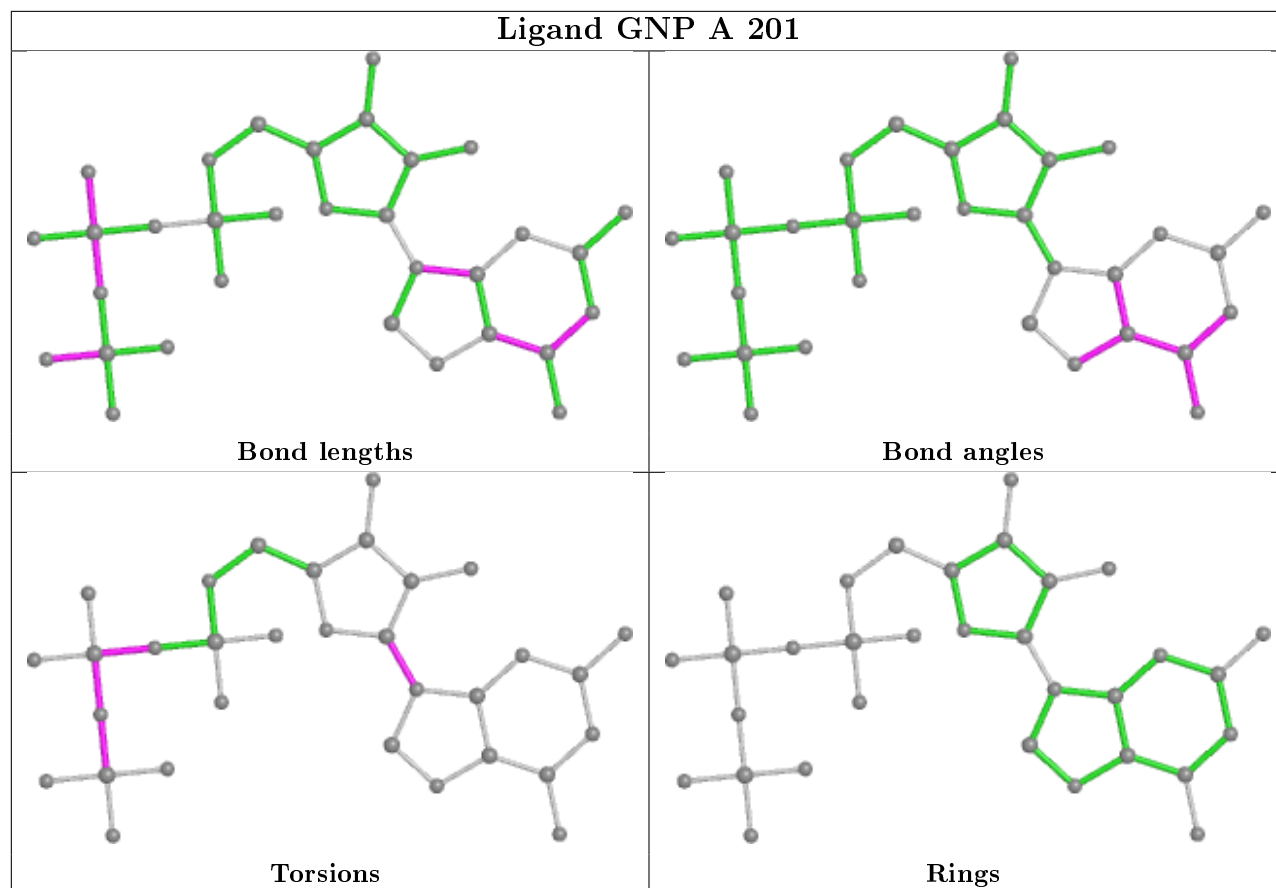
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	2005	FMT	1	0
7	C	201	FMT	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.





## 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	165/167 (98%)	-0.11	3 (1%) 68 72	13, 21, 42, 58	0
2	B	469/482 (97%)	-0.15	8 (1%) 70 74	11, 19, 38, 75	0
3	C	167/167 (100%)	0.22	16 (9%) 8 8	12, 21, 55, 91	0
All	All	801/816 (98%)	-0.06	27 (3%) 45 48	11, 19, 43, 91	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	0	GLY	6.5
3	C	29	VAL	5.1
3	C	120	LEU	5.1
3	C	26	ASN	4.9
3	C	27	HIS	4.9
2	B	751	ASN	4.3
3	C	37	GLU	3.9
3	C	38	ASP	3.7
2	B	565	GLY	3.7
3	C	121	ALA	3.6
3	C	122	ALA	3.1
3	C	48	GLY	2.9
3	C	166	HIS	2.8
2	B	597	GLY	2.7
2	B	1021	PRO	2.7
2	B	755	GLN	2.6
3	C	30	ASP	2.6
3	C	31	GLU	2.5
3	C	1	MET	2.5
2	B	574	VAL	2.4
2	B	670	LEU	2.4
1	A	105	ASP	2.4
3	C	39	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	49	GLU	2.2
1	A	107	ASP	2.2
2	B	573	ASP	2.1
1	A	1	MET	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSO	A	51	7/8	0.96	0.10	17,18,30,35	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

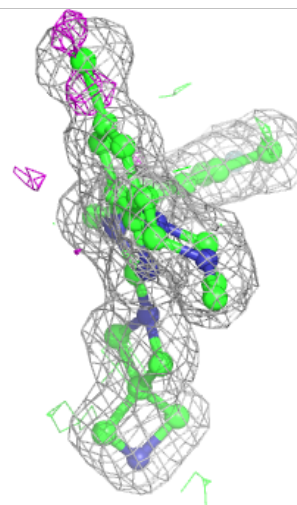
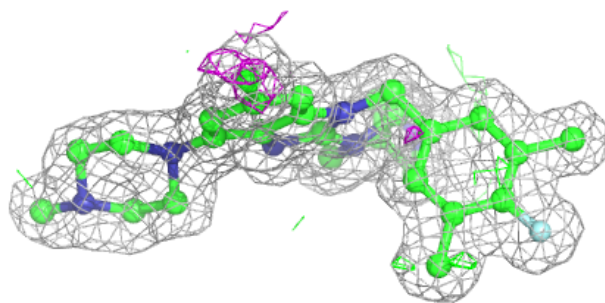
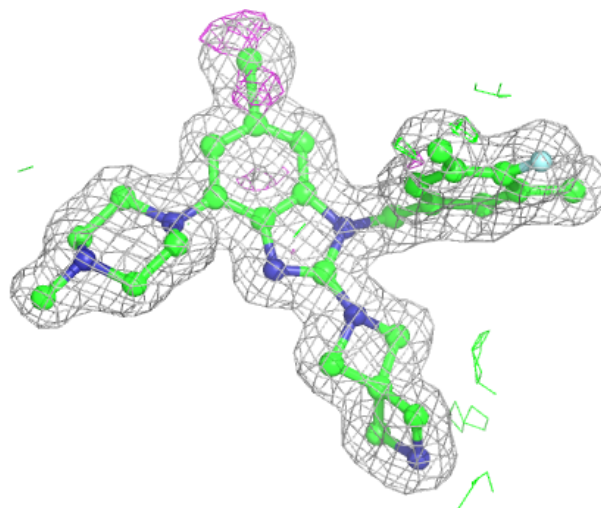
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

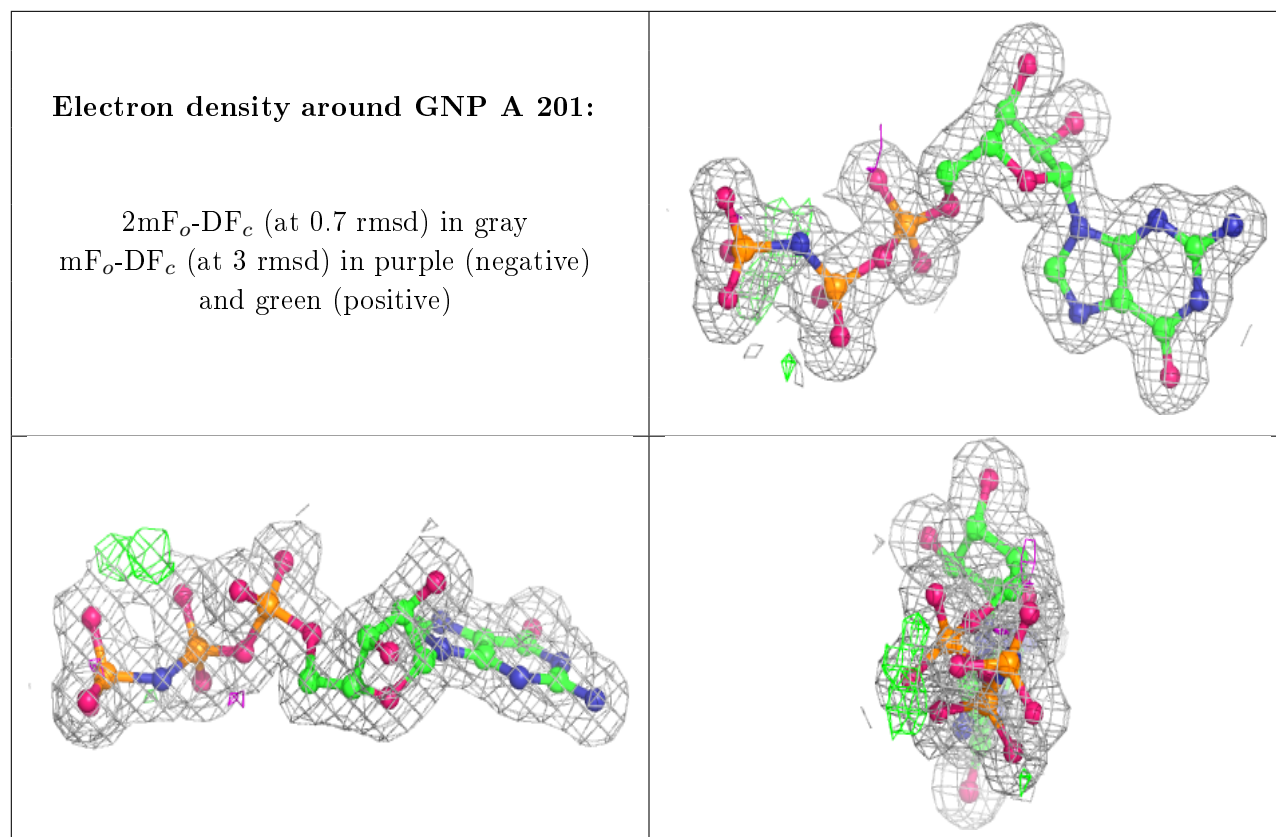
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	FMT	B	2006	3/3	0.74	0.23	64,64,68,69	0
7	FMT	B	2002	3/3	0.77	0.14	54,54,55,61	0
8	GOL	B	2007	6/6	0.85	0.17	25,44,58,61	0
7	FMT	B	2003	3/3	0.91	0.23	47,47,50,56	0
7	FMT	B	2005	3/3	0.92	0.16	22,22,23,31	0
7	FMT	B	2004	3/3	0.94	0.14	39,39,40,41	0
8	GOL	B	2008	6/6	0.94	0.11	26,37,45,49	0
7	FMT	C	201	3/3	0.94	0.12	29,29,35,39	0
6	FWA	B	2001	34/34	0.96	0.07	13,17,26,31	0
4	GNP	A	201	32/32	0.98	0.07	13,17,20,25	0
5	MG	A	202	1/1	0.99	0.11	10,10,10,10	0
9	NA	C	202	1/1	0.99	0.06	34,34,34,34	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 FWA B 2001:**

$2mF_o-DF_c$  (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.