



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 03:12 pm BST

PDB ID : 3X06  
Title : Crystal structure of PIP4KIIBETA T201M complex with GMP  
Authors : Takeuchi, K.; Lo, Y.H.; Sumita, K.; Senda, M.; Terakawa, J.; Dimitoris, A.; Locasale, J.W.; Sasaki, M.; Yoshino, H.; Zhang, Y.; Kahoud, E.R.; Takano, T.; Yokota, T.; Emerling, B.; Asara, J.A.; Ishida, T.; Shimada, I.; Daikoku, T.; Cantley, L.C.; Senda, T.; Sasaki, A.T.  
Deposited on : 2014-10-09  
Resolution : 2.65 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 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

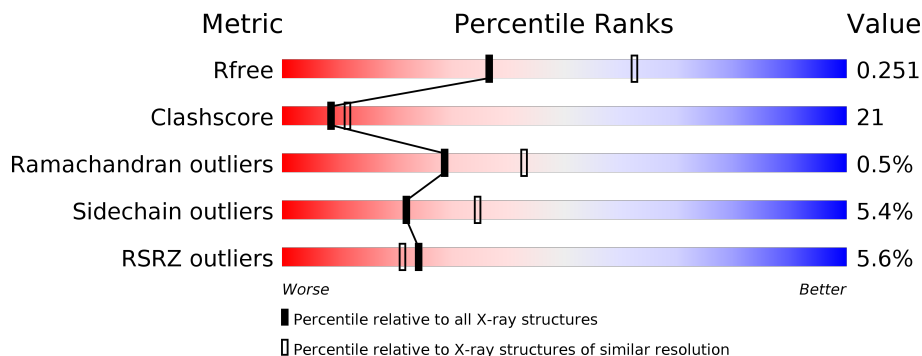
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	393	
1	B	393	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5324 atoms, of which 60 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.

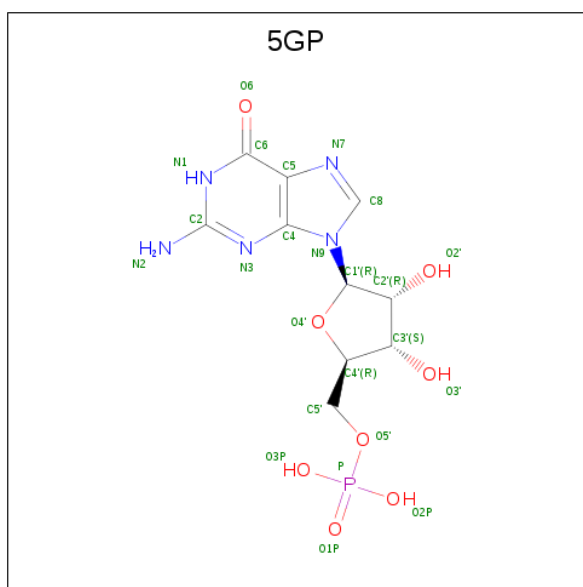
- Molecule 1 is a protein called Phosphatidylinositol 5-phosphate 4-kinase type-2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	318	2617	1666	446	490	15	0	0	0
1	B	303	2496	1599	426	457	14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	EXPRESSION TAG	UNP P78356
A	25	PRO	-	EXPRESSION TAG	UNP P78356
A	26	ASN	-	EXPRESSION TAG	UNP P78356
A	27	CYS	-	EXPRESSION TAG	UNP P78356
A	28	ALA	-	EXPRESSION TAG	UNP P78356
A	29	PRO	-	EXPRESSION TAG	UNP P78356
A	30	GLY	-	EXPRESSION TAG	UNP P78356
A	201	MET	THR	ENGINEERED MUTATION	UNP P78356
B	24	GLY	-	EXPRESSION TAG	UNP P78356
B	25	PRO	-	EXPRESSION TAG	UNP P78356
B	26	ASN	-	EXPRESSION TAG	UNP P78356
B	27	CYS	-	EXPRESSION TAG	UNP P78356
B	28	ALA	-	EXPRESSION TAG	UNP P78356
B	29	PRO	-	EXPRESSION TAG	UNP P78356
B	30	GLY	-	EXPRESSION TAG	UNP P78356
B	201	MET	THR	ENGINEERED MUTATION	UNP P78356

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	Total	C	H	N	O	P	0	0
			36	10	12	5	8	1		
2	A	1	Total	C	H	N	O	P	0	0
			36	10	12	5	8	1		
2	A	1	Total	C	H	N	O	P	0	0
			36	10	12	5	8	1		
2	A	1	Total	C	H	N	O	P	0	0
			36	10	12	5	8	1		
2	B	1	Total	C	H	N	O	P	0	0
			36	10	12	5	8	1		

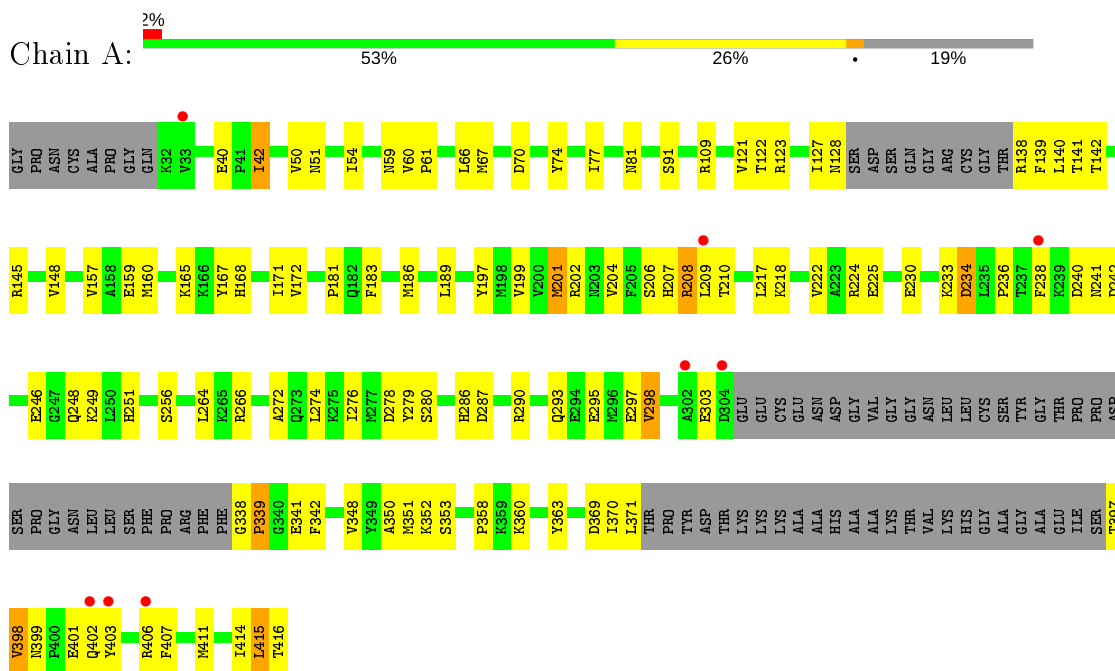
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	14	Total	O	0	0
			14	14		

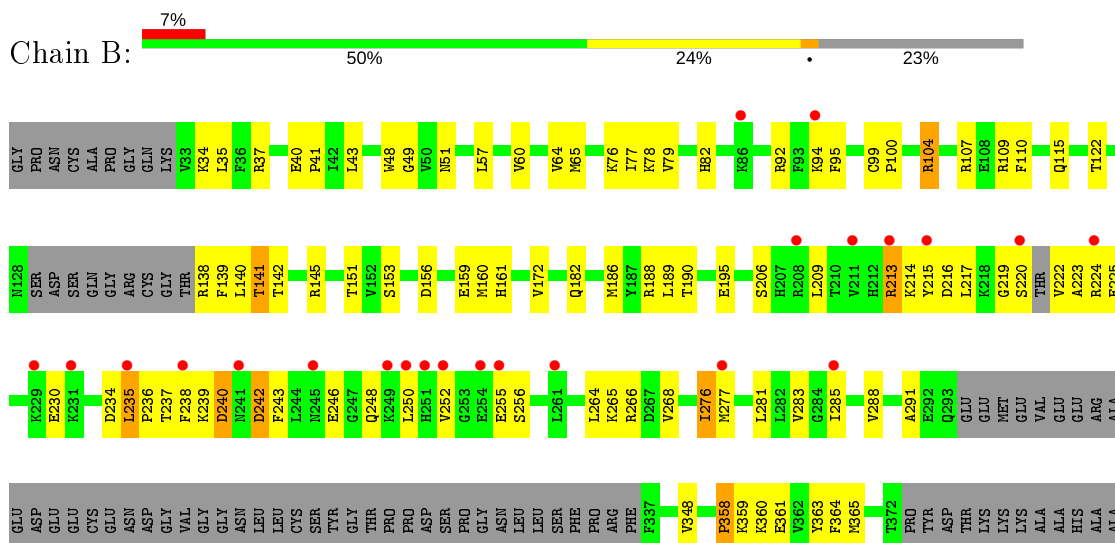
### 3 Residue-property plots

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: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta



- Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta



LYS	
THR	
VAL	
LYS	
HIS	
GLY	
ALA	
GLY	
ALA	
GLU	
ILE	
SER	
THR	
VAL	
ASN	
P400	
R406	●
F407	
H408	
E409	
F410	
M411	●
S412	
H413	●
L414	●
L415	
THR	

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.83Å 182.88Å 106.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.41 – 2.65 91.44 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (54.41-2.65) 99.0 (91.44-2.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 2.65Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, $R_{free}$	0.212 , 0.261 0.199 , 0.251	Depositor DCC
$R_{free}$ test set	1549 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 73.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.019 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5324	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: 5GP

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	0.46	0/2670	0.56	0/3590
1	B	0.46	1/2549 (0.0%)	0.55	1/3426 (0.0%)
All	All	0.46	1/5219 (0.0%)	0.55	1/7016 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	GLU	C-N	-5.75	1.20	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	255	GLU	O-C-N	5.13	130.91	122.70

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	2617	0	2591	102	0
1	B	2496	0	2482	121	0
2	A	96	48	48	2	0
2	B	24	12	12	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	17	0	0	0	0
3	B	14	0	0	1	0
All	All	5264	60	5133	214	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 21.

All (214) 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:399:ASN:OD1	1:A:402:GLN:HG2	1.35	1.23
1:B:235:LEU:H	1:B:235:LEU:HD12	1.12	1.13
1:B:243:PHE:HE2	1:B:414:ILE:CG2	1.63	1.10
1:B:243:PHE:CE2	1:B:414:ILE:CG2	2.45	0.99
1:A:141:THR:HG22	1:A:142:THR:O	1.65	0.95
1:B:236:PRO:HB2	1:B:238:PHE:CE1	2.03	0.94
1:B:222:VAL:HG12	1:B:223:ALA:H	1.29	0.94
1:B:243:PHE:CE2	1:B:414:ILE:HG21	2.03	0.93
1:B:277:MET:SD	1:B:400:PRO:N	2.42	0.92
1:B:213:ARG:CG	1:B:215:TYR:CE1	2.53	0.92
1:A:77:ILE:HD11	1:B:77:ILE:HD11	1.50	0.92
1:A:217:LEU:HD13	1:A:414:ILE:HD11	1.54	0.90
1:A:399:ASN:OD1	1:A:402:GLN:CG	2.20	0.88
1:B:243:PHE:HE2	1:B:414:ILE:HG22	1.40	0.86
1:B:141:THR:HG22	1:B:142:THR:O	1.76	0.84
1:B:235:LEU:N	1:B:235:LEU:HD12	1.93	0.82
1:B:213:ARG:HG3	1:B:215:TYR:CE1	2.15	0.81
1:A:398:VAL:HG12	1:A:402:GLN:HG3	1.63	0.80
1:B:213:ARG:CG	1:B:215:TYR:HE1	1.91	0.80
1:A:225:GLU:HG3	1:A:241:ASN:HB2	1.65	0.79
1:B:110:PHE:CE1	1:B:182:GLN:HG2	2.18	0.78
1:B:219:GLY:HA2	1:B:410:PHE:CD2	2.19	0.78
1:A:338:GLY:N	1:A:339:PRO:HD3	2.00	0.77
1:A:77:ILE:CD1	1:B:77:ILE:HD11	2.16	0.75
1:B:281:LEU:HD22	1:B:411:MET:CG	2.15	0.75
1:A:242:ASP:O	1:A:246:GLU:HG3	1.87	0.74
1:A:189:LEU:N	1:A:189:LEU:HD12	2.03	0.73
1:A:338:GLY:N	1:A:339:PRO:CD	2.53	0.72
1:A:77:ILE:HD12	1:B:79:VAL:HG22	1.72	0.72
1:A:256:SER:HB3	1:A:351:MET:HE1	1.71	0.71
1:B:213:ARG:HG2	1:B:215:TYR:CE1	2.23	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ASP:O	1:B:246:GLU:HG3	1.91	0.71
1:B:235:LEU:H	1:B:235:LEU:CD1	1.95	0.71
1:A:77:ILE:HD11	1:B:77:ILE:CD1	2.21	0.70
1:B:78:LYS:HD2	1:B:94:LYS:HE2	1.73	0.70
1:A:128:ASN:HB3	1:A:140:LEU:HD23	1.74	0.70
1:B:141:THR:CG2	1:B:145:ARG:HA	2.21	0.70
1:A:181:PRO:HB3	1:A:201:MET:HE2	1.73	0.69
1:A:217:LEU:HD13	1:A:414:ILE:CD1	2.23	0.68
1:A:141:THR:HG23	1:A:145:ARG:HA	1.76	0.68
1:A:224:ARG:NH1	1:A:240:ASP:OD1	2.24	0.68
1:B:43:LEU:HD21	1:B:140:LEU:HD11	1.76	0.68
1:B:141:THR:HG23	1:B:145:ARG:HA	1.75	0.68
1:A:218:LYS:HD2	1:A:224:ARG:NE	2.08	0.67
1:B:94:LYS:HB2	1:B:190:THR:HB	1.76	0.67
1:A:256:SER:HB3	1:A:351:MET:CE	2.24	0.67
1:A:42:ILE:H	1:A:42:ILE:HD13	1.60	0.66
1:A:42:ILE:HD13	1:A:42:ILE:N	2.10	0.66
1:B:216:ASP:C	1:B:217:LEU:HD23	2.16	0.66
1:A:183:PHE:CE1	1:A:201:MET:HE3	2.29	0.66
1:B:109:ARG:CZ	1:B:172:VAL:HG22	2.25	0.66
1:B:243:PHE:CE2	1:B:414:ILE:HG22	2.22	0.66
1:A:141:THR:CG2	1:A:145:ARG:HA	2.26	0.66
1:B:281:LEU:HD22	1:B:411:MET:HG3	1.77	0.66
1:A:77:ILE:CG1	1:B:77:ILE:HD11	2.25	0.65
1:A:398:VAL:HA	1:A:402:GLN:OE1	1.96	0.65
1:B:406:ARG:HG2	1:B:407:PHE:N	2.10	0.64
1:B:250:LEU:HB2	1:B:415:LEU:HD23	1.79	0.64
1:B:216:ASP:O	1:B:217:LEU:HD23	1.97	0.64
1:A:217:LEU:CD1	1:A:414:ILE:CD1	2.75	0.64
1:B:222:VAL:HG12	1:B:223:ALA:N	2.08	0.64
1:A:51:ASN:HB2	1:A:122:THR:HG21	1.81	0.63
1:B:242:ASP:N	1:B:242:ASP:OD1	2.29	0.63
1:B:213:ARG:HG2	1:B:215:TYR:HE1	1.63	0.63
1:B:214:LYS:HG3	1:B:237:THR:HA	1.81	0.63
1:A:138:ARG:HD3	1:A:140:LEU:HD11	1.80	0.62
1:A:138:ARG:HG2	1:A:139:PHE:N	2.15	0.62
1:B:159:GLU:HA	1:B:159:GLU:OE2	1.97	0.62
1:A:217:LEU:CD1	1:A:414:ILE:HD11	2.29	0.62
1:B:213:ARG:NH2	1:B:238:PHE:HE1	1.98	0.62
1:A:341:GLU:HG3	1:A:342:PHE:N	2.15	0.61
1:A:279:TYR:HB3	1:A:369:ASP:O	2.01	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LEU:HD21	1:B:140:LEU:CD1	2.29	0.61
1:A:411:MET:HA	1:A:414:ILE:HD12	1.82	0.60
1:B:60:VAL:O	1:B:104:ARG:NH2	2.34	0.60
1:B:79:VAL:O	1:B:92:ARG:HA	2.01	0.60
1:B:161:HIS:HE1	3:B:606:HOH:O	1.83	0.60
1:A:341:GLU:OE2	1:A:352:LYS:HD2	2.01	0.60
1:A:339:PRO:O	1:A:360:LYS:NZ	2.35	0.59
1:A:341:GLU:HG3	1:A:342:PHE:H	1.68	0.59
1:B:213:ARG:HG2	1:B:215:TYR:OH	2.01	0.59
1:B:240:ASP:N	1:B:240:ASP:OD1	2.32	0.59
1:A:42:ILE:H	1:A:42:ILE:CD1	2.14	0.58
1:B:189:LEU:HD12	1:B:189:LEU:N	2.19	0.58
1:B:51:ASN:HB2	1:B:122:THR:HG21	1.84	0.58
1:A:399:ASN:H	1:A:402:GLN:CG	2.17	0.58
1:B:288:VAL:O	1:B:291:ALA:HB3	2.03	0.57
1:A:181:PRO:HB3	1:A:201:MET:CE	2.34	0.57
1:B:35:LEU:HD13	1:B:37:ARG:NH2	2.18	0.57
1:B:219:GLY:CA	1:B:410:PHE:CD2	2.87	0.57
1:A:109:ARG:CZ	1:A:172:VAL:HG22	2.34	0.57
1:B:213:ARG:NH2	1:B:238:PHE:CE1	2.72	0.56
1:B:264:LEU:HD11	1:B:407:PHE:HE1	1.70	0.56
1:A:139:PHE:CZ	1:A:148:VAL:HG11	2.40	0.56
1:A:66:LEU:HD12	1:A:168:HIS:CE1	2.40	0.56
1:B:78:LYS:HD2	1:B:94:LYS:CE	2.35	0.56
1:B:206:SER:HB2	1:B:364:PHE:CE2	2.41	0.56
1:B:214:LYS:HG3	1:B:236:PRO:O	2.06	0.56
1:A:138:ARG:CG	1:A:139:PHE:N	2.69	0.55
1:A:186:MET:HG3	1:A:199:VAL:HG22	1.88	0.55
1:B:225:GLU:HA	1:B:242:ASP:OD1	2.07	0.55
1:B:213:ARG:CB	1:B:215:TYR:HE1	2.19	0.55
1:B:243:PHE:CE1	1:B:248:GLN:HG2	2.42	0.55
1:A:183:PHE:CE1	1:A:201:MET:CE	2.90	0.55
1:B:213:ARG:CG	1:B:215:TYR:CZ	2.89	0.55
1:A:40:GLU:OE1	1:A:138:ARG:NH2	2.41	0.54
1:B:153:SER:O	1:B:156:ASP:HB2	2.07	0.54
1:A:236:PRO:HB2	1:A:238:PHE:CE2	2.42	0.54
1:A:264:LEU:HD11	1:A:407:PHE:HE1	1.73	0.54
1:A:415:LEU:H	1:A:415:LEU:HD23	1.73	0.54
1:A:160:MET:HG2	1:A:186:MET:SD	2.48	0.53
1:A:50:VAL:O	1:A:54:ILE:HG12	2.09	0.53
1:B:49:GLY:HA3	1:B:95:PHE:CE1	2.44	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:THR:CG2	1:B:142:THR:O	2.54	0.52
1:B:214:LYS:CG	1:B:236:PRO:O	2.57	0.52
1:B:48:TRP:HH2	1:B:77:ILE:HD13	1.75	0.52
1:B:206:SER:CB	1:B:209:LEU:HB2	2.40	0.52
1:B:213:ARG:HG2	1:B:215:TYR:CZ	2.44	0.52
1:A:139:PHE:CZ	1:A:148:VAL:CG1	2.93	0.51
1:A:217:LEU:CD1	1:A:414:ILE:HD13	2.38	0.51
1:A:50:VAL:HG21	1:A:121:VAL:HG11	1.93	0.51
1:B:220:SER:CB	1:B:406:ARG:HD3	2.41	0.51
1:B:213:ARG:HB3	1:B:215:TYR:HE1	1.75	0.51
1:B:213:ARG:HG3	1:B:215:TYR:CZ	2.44	0.51
1:B:189:LEU:CD1	1:B:189:LEU:N	2.73	0.51
1:B:407:PHE:C	1:B:407:PHE:CD1	2.84	0.51
1:B:243:PHE:HE2	1:B:414:ILE:CB	2.23	0.50
1:B:243:PHE:HE1	1:B:248:GLN:HG2	1.74	0.50
1:A:183:PHE:CD1	1:A:201:MET:HE3	2.46	0.50
1:A:217:LEU:HD12	1:A:414:ILE:HD13	1.94	0.50
1:B:206:SER:HB3	1:B:209:LEU:HB2	1.95	0.49
1:A:204:VAL:HG23	2:A:501:5GP:O6	2.12	0.49
1:A:138:ARG:HD3	1:A:140:LEU:CG	2.43	0.49
1:B:188:ARG:C	1:B:189:LEU:HD12	2.32	0.49
1:B:277:MET:SD	1:B:400:PRO:CD	3.00	0.49
1:A:234:ASP:N	1:A:234:ASP:OD1	2.45	0.49
1:A:189:LEU:N	1:A:189:LEU:CD1	2.73	0.49
1:A:206:SER:HB3	1:A:209:LEU:HB2	1.95	0.49
1:A:138:ARG:HD3	1:A:140:LEU:CD1	2.43	0.48
1:A:157:VAL:HG21	1:A:197:TYR:CD1	2.48	0.48
1:B:222:VAL:CG1	1:B:223:ALA:H	2.12	0.48
1:B:213:ARG:CG	1:B:215:TYR:OH	2.62	0.48
1:B:252:VAL:CG2	1:B:256:SER:HB2	2.43	0.48
1:A:67:MET:O	1:A:70:ASP:HB2	2.14	0.48
1:B:409:GLU:O	1:B:412:SER:N	2.47	0.47
1:A:230:GLU:OE1	1:A:233:LYS:HD2	2.13	0.47
1:B:288:VAL:HG23	1:B:360:LYS:O	2.14	0.47
1:B:243:PHE:CE1	1:B:248:GLN:HB3	2.50	0.47
1:B:99:CYS:N	1:B:100:PRO:HD3	2.30	0.47
1:A:141:THR:CG2	1:A:142:THR:O	2.52	0.46
1:B:104:ARG:HA	1:B:107:ARG:NH1	2.30	0.46
1:A:59:ASN:HB3	1:B:34:LYS:O	2.15	0.46
1:B:220:SER:HB2	1:B:406:ARG:HD3	1.97	0.46
1:B:110:PHE:CZ	1:B:182:GLN:HG2	2.49	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:HG23	1:B:256:SER:HB2	1.96	0.46
1:A:415:LEU:H	1:A:415:LEU:CD2	2.27	0.46
1:A:293:GLN:OE1	2:A:502:5GP:C6	2.64	0.46
1:A:251:HIS:O	1:A:353:SER:HA	2.16	0.46
1:A:248:GLN:HG3	1:A:249:LYS:N	2.30	0.46
1:B:358:PRO:HB2	1:B:359:LYS:H	1.60	0.45
1:A:415:LEU:C	1:A:416:THR:HG23	2.36	0.45
1:A:74:TYR:CE2	1:B:82:HIS:CB	2.99	0.45
1:A:159:GLU:HA	1:A:159:GLU:OE2	2.16	0.45
1:B:234:ASP:O	1:B:236:PRO:HD3	2.16	0.45
1:B:250:LEU:HD12	1:B:415:LEU:HD21	1.98	0.45
1:A:74:TYR:CZ	1:B:82:HIS:HB2	2.51	0.45
1:A:218:LYS:HD2	1:A:224:ARG:CZ	2.47	0.45
1:B:214:LYS:HE2	1:B:214:LYS:HB3	1.83	0.44
1:A:295:GLU:O	1:A:298:VAL:HG12	2.17	0.44
1:B:264:LEU:O	1:B:268:VAL:HG22	2.17	0.44
1:A:415:LEU:O	1:A:416:THR:CG2	2.66	0.44
1:B:237:THR:HG22	1:B:237:THR:O	2.17	0.44
1:A:81:ASN:O	1:A:91:SER:HB3	2.17	0.44
1:A:207:HIS:CE1	1:A:208:ARG:HG2	2.52	0.44
1:A:370:ILE:O	1:A:370:ILE:HG13	2.18	0.44
1:A:287:ASP:HB3	1:A:290:ARG:HB3	1.99	0.43
1:B:276:ILE:HG22	1:B:277:MET:N	2.33	0.43
1:A:415:LEU:O	1:A:416:THR:HG23	2.18	0.43
1:A:341:GLU:CG	1:A:342:PHE:H	2.30	0.43
1:A:74:TYR:CE2	1:B:82:HIS:HB3	2.53	0.43
1:B:220:SER:HB3	1:B:406:ARG:HD3	2.01	0.43
1:B:348:VAL:HG12	1:B:348:VAL:O	2.19	0.42
1:B:250:LEU:HD12	1:B:415:LEU:CD2	2.50	0.42
1:A:350:ALA:HA	1:A:363:TYR:O	2.19	0.42
1:B:43:LEU:CD2	1:B:140:LEU:CD1	2.97	0.42
1:A:230:GLU:CD	1:A:233:LYS:HD2	2.40	0.42
1:B:215:TYR:HB3	1:B:217:LEU:HD21	2.00	0.42
1:B:139:PHE:CD1	1:B:139:PHE:O	2.72	0.42
1:A:186:MET:HG3	1:A:199:VAL:CG2	2.50	0.42
1:A:272:ALA:O	1:A:274:LEU:O	2.38	0.41
1:A:407:PHE:O	1:A:411:MET:HG2	2.20	0.41
1:B:40:GLU:HA	1:B:41:PRO:HD3	1.89	0.41
1:A:210:THR:O	1:A:286:HIS:ND1	2.45	0.41
1:B:240:ASP:HB3	1:B:410:PHE:CZ	2.55	0.41
1:A:341:GLU:CG	1:A:342:PHE:N	2.83	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LEU:O	1:B:195:GLU:HA	2.21	0.41
1:A:202:ARG:CZ	1:A:348:VAL:HG21	2.51	0.41
1:B:283:VAL:HG22	1:B:365:MET:HG2	2.02	0.41
1:B:215:TYR:CD2	1:B:238:PHE:HB2	2.56	0.41
1:B:57:LEU:O	1:B:104:ARG:NH2	2.54	0.41
1:A:234:ASP:O	1:A:236:PRO:HD3	2.21	0.41
1:B:138:ARG:HG3	1:B:151:THR:OG1	2.21	0.41
1:B:160:MET:HG2	1:B:186:MET:SD	2.60	0.41
1:B:213:ARG:HB2	1:B:285:ILE:HB	2.02	0.41
1:A:274:LEU:HB2	1:A:276:ILE:HG12	2.03	0.41
1:B:240:ASP:HB3	1:B:410:PHE:CE2	2.56	0.41
1:A:293:GLN:O	1:A:297:GLU:HG3	2.21	0.41
1:A:278:ASP:HA	1:A:403:TYR:CZ	2.57	0.40
1:A:60:VAL:HA	1:A:61:PRO:HD2	1.86	0.40
1:B:361:GLU:HG3	1:B:363:TYR:CZ	2.56	0.40
1:B:141:THR:HG21	1:B:145:ARG:HA	1.98	0.40
1:B:64:VAL:HG23	1:B:65:MET:HG2	2.02	0.40
1:A:167:TYR:O	1:A:171:ILE:HG12	2.21	0.40
1:B:224:ARG:HB3	1:B:239:LYS:HD3	2.03	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	Percentiles	
1	A	310/393 (79%)	297 (96%)	11 (4%)	2 (1%)	25	37
1	B	293/393 (75%)	283 (97%)	9 (3%)	1 (0%)	41	56
All	All	603/786 (77%)	580 (96%)	20 (3%)	3 (0%)	29	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	PRO
1	A	358	PRO
1	B	358	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/352 (84%)	277 (94%)	18 (6%)	18	29
1	B	281/352 (80%)	268 (95%)	13 (5%)	27	41
All	All	576/704 (82%)	545 (95%)	31 (5%)	22	34

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ILE
1	A	123	ARG
1	A	127	ILE
1	A	165	LYS
1	A	201	MET
1	A	208	ARG
1	A	222	VAL
1	A	234	ASP
1	A	266	ARG
1	A	280	SER
1	A	298	VAL
1	A	303	GLU
1	A	371	LEU
1	A	397	THR
1	A	398	VAL
1	A	401	GLU
1	A	406	ARG
1	A	415	LEU
1	B	76	LYS
1	B	104	ARG
1	B	115	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	141	THR
1	B	213	ARG
1	B	230	GLU
1	B	235	LEU
1	B	240	ASP
1	B	242	ASP
1	B	265	LYS
1	B	266	ARG
1	B	276	ILE
1	B	411	MET

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are 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
2	5GP	A	501	-	22,26,26	0.51	0	27,40,40	1.79	6 (22%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	5GP	A	504	-	22,26,26	0.65	0	27,40,40	1.85	7 (25%)
2	5GP	A	503	-	22,26,26	0.57	0	27,40,40	1.86	7 (25%)
2	5GP	A	502	-	22,26,26	1.84	11 (50%)	27,40,40	1.98	8 (29%)
2	5GP	B	501	-	22,26,26	0.51	0	27,40,40	1.75	5 (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
2	5GP	A	501	-	-	4/6/26/26	0/3/3/3
2	5GP	A	504	-	-	3/6/26/26	0/3/3/3
2	5GP	A	503	-	-	0/6/26/26	0/3/3/3
2	5GP	A	502	-	-	0/6/26/26	0/3/3/3
2	5GP	B	501	-	-	6/6/26/26	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	5GP	C2'-C1'	-2.63	1.49	1.53
2	A	502	5GP	P-O3P	-2.63	1.44	1.54
2	A	502	5GP	C2-N1	-2.57	1.30	1.35
2	A	502	5GP	P-O2P	-2.51	1.45	1.54
2	A	502	5GP	C6-C5	2.40	1.45	1.41
2	A	502	5GP	O4'-C4'	-2.38	1.39	1.45
2	A	502	5GP	C4-N3	-2.23	1.32	1.35
2	A	502	5GP	C2'-C3'	-2.17	1.47	1.53
2	A	502	5GP	P-O5'	-2.11	1.53	1.60
2	A	502	5GP	P-O1P	-2.08	1.43	1.50
2	A	502	5GP	C3'-C4'	-2.06	1.47	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	5GP	C2-N3-C4	5.10	121.18	115.36
2	A	504	5GP	N3-C2-N1	-5.04	120.50	127.22
2	A	504	5GP	C2-N3-C4	4.98	121.05	115.36
2	A	503	5GP	N3-C2-N1	-4.80	120.82	127.22
2	A	502	5GP	C2-N3-C4	4.73	120.76	115.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	5GP	N3-C2-N1	-4.44	121.29	127.22
2	B	501	5GP	N3-C2-N1	-4.40	121.35	127.22
2	A	501	5GP	C2-N3-C4	4.12	120.06	115.36
2	A	502	5GP	C6-C5-C4	-3.97	117.01	120.80
2	B	501	5GP	C2-N3-C4	3.79	119.69	115.36
2	A	502	5GP	C4-C5-N7	-3.60	105.64	109.40
2	B	501	5GP	C6-N1-C2	3.41	121.35	115.93
2	A	501	5GP	C6-N1-C2	3.34	121.23	115.93
2	A	502	5GP	C5-C6-N1	-3.28	118.94	123.43
2	A	501	5GP	C5-C6-N1	-3.11	119.17	123.43
2	B	501	5GP	C5-C6-N1	-3.11	119.18	123.43
2	A	502	5GP	C6-N1-C2	3.09	120.84	115.93
2	A	503	5GP	O3P-P-O5'	-2.90	99.03	106.73
2	A	501	5GP	O3P-P-O5'	-2.87	99.10	106.73
2	A	503	5GP	C6-N1-C2	2.76	120.31	115.93
2	A	504	5GP	C6-N1-C2	2.70	120.21	115.93
2	A	503	5GP	C5-C6-N1	-2.62	119.85	123.43
2	A	502	5GP	O2P-P-O5'	-2.51	100.06	106.73
2	A	504	5GP	C5-C6-N1	-2.50	120.02	123.43
2	A	504	5GP	O3P-P-O5'	-2.43	100.27	106.73
2	A	502	5GP	O3P-P-O1P	2.40	120.07	110.68
2	A	504	5GP	C4-C5-N7	-2.37	106.92	109.40
2	B	501	5GP	C4-C5-N7	-2.36	106.94	109.40
2	A	501	5GP	C4-C5-N7	-2.32	106.98	109.40
2	A	502	5GP	N3-C2-N1	-2.27	124.20	127.22
2	A	503	5GP	N2-C2-N1	2.12	120.55	117.25
2	A	503	5GP	C4-C5-N7	-2.11	107.20	109.40
2	A	504	5GP	N2-C2-N1	2.02	120.40	117.25

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	5GP	C5'-O5'-P-O2P
2	B	501	5GP	C5'-O5'-P-O3P
2	A	504	5GP	C5'-O5'-P-O1P
2	A	504	5GP	C5'-O5'-P-O2P
2	A	504	5GP	C5'-O5'-P-O3P
2	A	501	5GP	C5'-O5'-P-O1P
2	A	501	5GP	C5'-O5'-P-O2P
2	A	501	5GP	C5'-O5'-P-O3P
2	A	501	5GP	C4'-C5'-O5'-P

*Continued on next page...*

Continued from previous page...

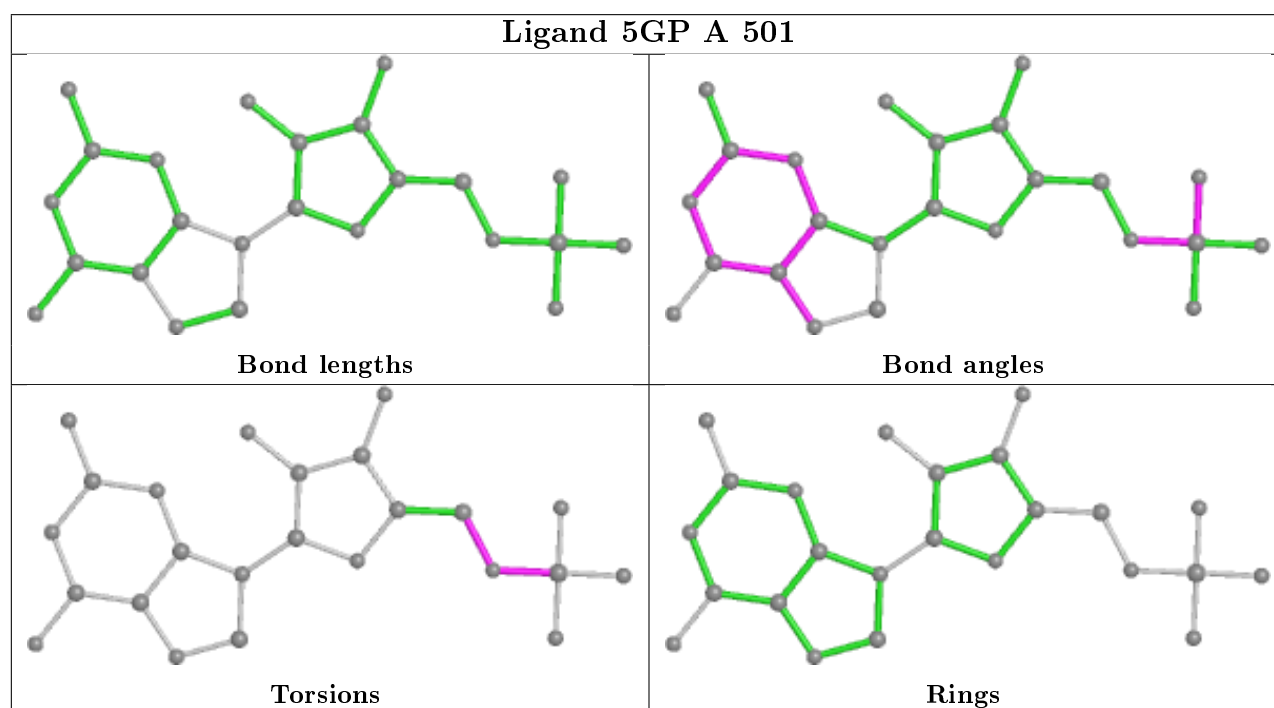
Mol	Chain	Res	Type	Atoms
2	B	501	5GP	C3'-C4'-C5'-O5'
2	B	501	5GP	O4'-C4'-C5'-O5'
2	B	501	5GP	C5'-O5'-P-O1P
2	B	501	5GP	C4'-C5'-O5'-P

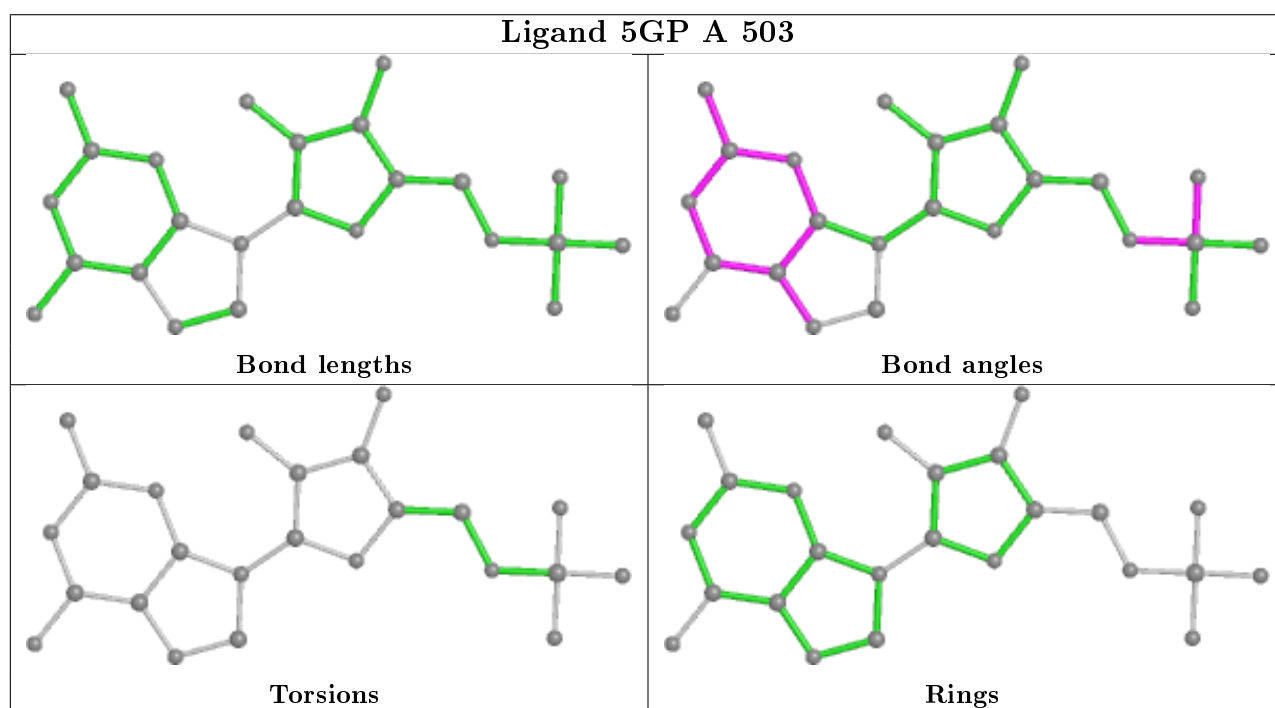
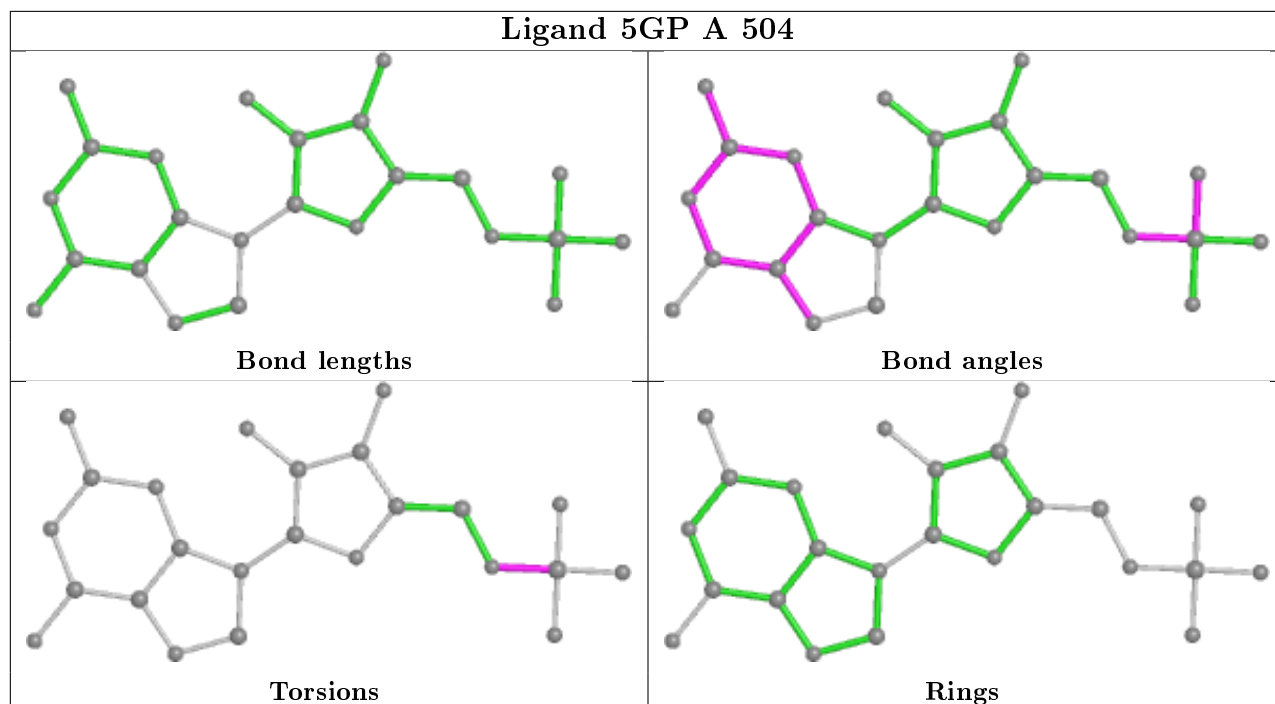
There are no ring outliers.

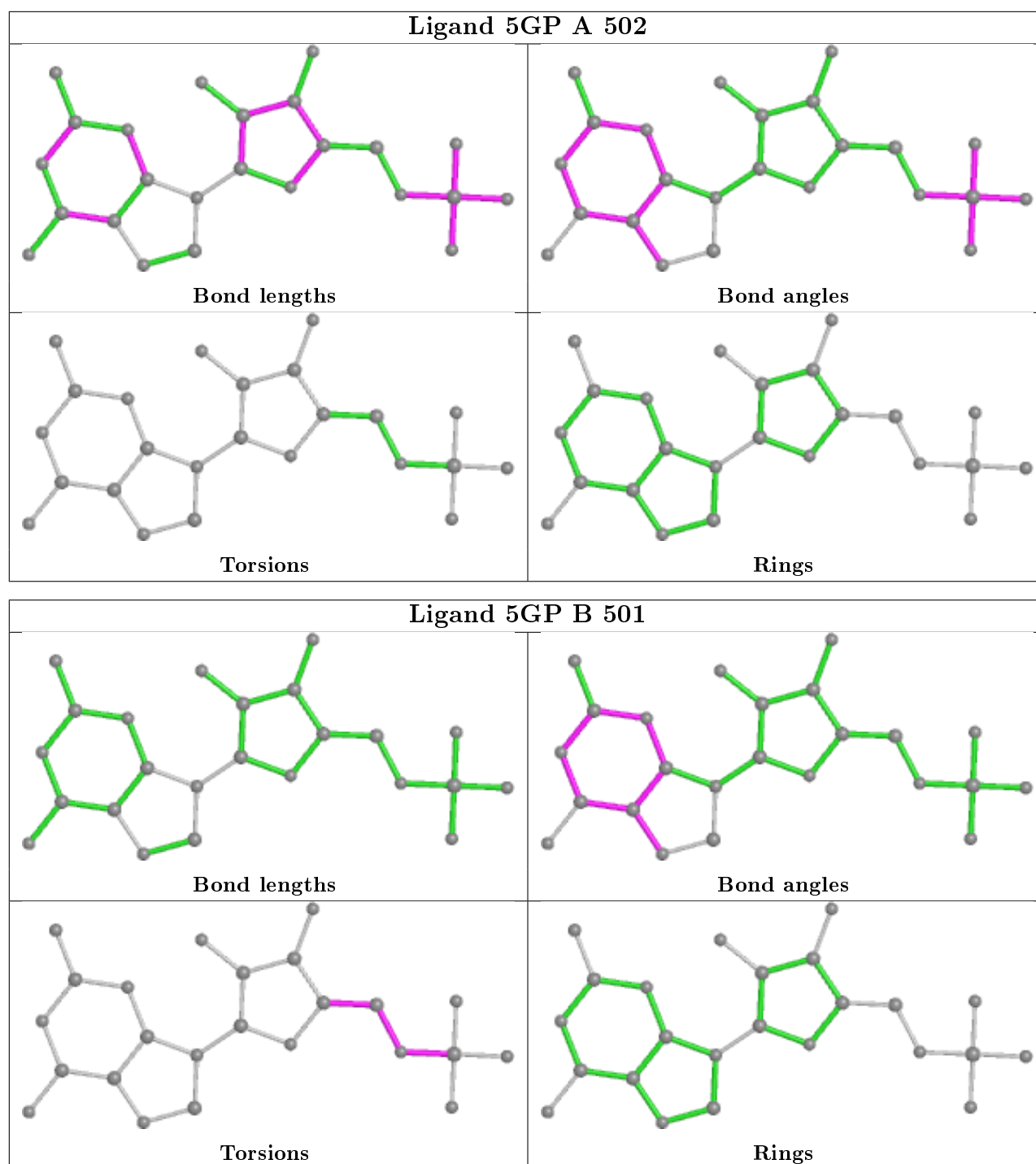
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	5GP	1	0
2	A	502	5GP	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	318/393 (80%)	0.59	8 (2%) 57 53	38, 70, 122, 158	0
1	B	303/393 (77%)	0.84	27 (8%) 9 8	38, 76, 143, 160	0
All	All	621/786 (79%)	0.71	35 (5%) 24 21	38, 73, 137, 160	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	415	LEU	5.3
1	B	250	LEU	5.0
1	B	414	ILE	4.1
1	A	304	ASP	4.0
1	B	213	ARG	3.8
1	B	249	LYS	3.7
1	B	215	TYR	3.6
1	B	220	SER	3.6
1	B	254	GLU	3.5
1	B	241	ASN	3.3
1	B	224	ARG	3.3
1	B	261	LEU	3.1
1	A	402	GLN	3.0
1	A	406	ARG	3.0
1	B	235	LEU	2.9
1	A	302	ALA	2.8
1	B	238	PHE	2.8
1	B	231	LYS	2.7
1	B	413	ASN	2.7
1	B	251	HIS	2.6
1	B	245	ASN	2.5
1	B	86	LYS	2.4
1	A	238	PHE	2.4
1	B	229	LYS	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	208	ARG	2.3
1	B	285	ILE	2.3
1	B	255	GLU	2.3
1	B	211	VAL	2.3
1	A	403	TYR	2.2
1	A	209	LEU	2.2
1	A	33	VAL	2.2
1	B	277	MET	2.2
1	B	94	LYS	2.2
1	B	252	VAL	2.1
1	B	411	MET	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

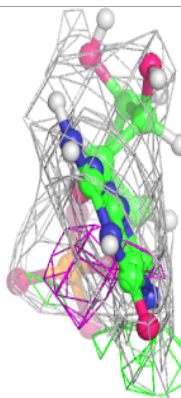
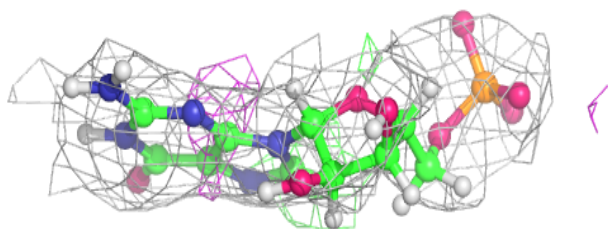
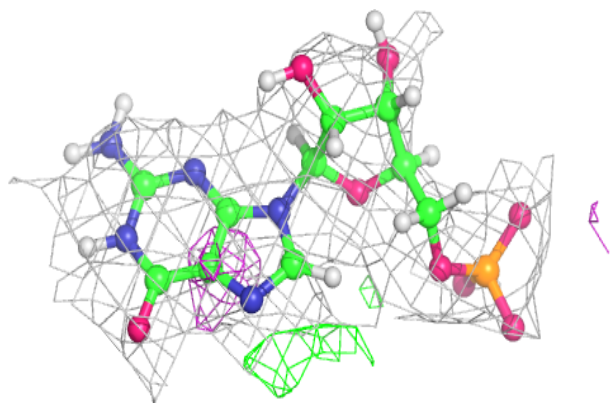
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
2	5GP	A	501	24/24	0.79	0.26	72,149,195,202	0
2	5GP	B	501	24/24	0.81	0.28	97,157,195,203	0
2	5GP	A	503	24/24	0.86	0.22	70,111,175,180	0
2	5GP	A	502	24/24	0.92	0.21	65,83,102,118	0
2	5GP	A	504	24/24	0.94	0.21	54,77,95,100	0

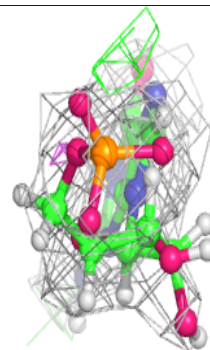
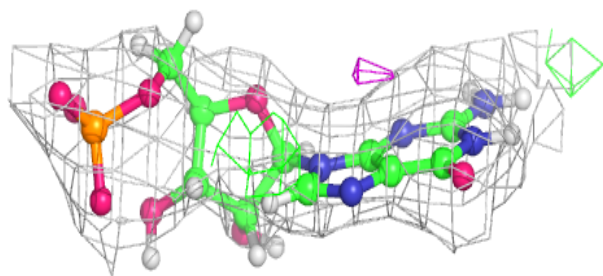
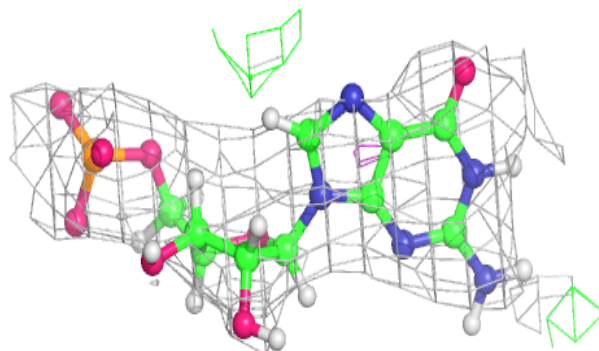
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 5GP A 501:**

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

**Electron density around 5GP B 501:**

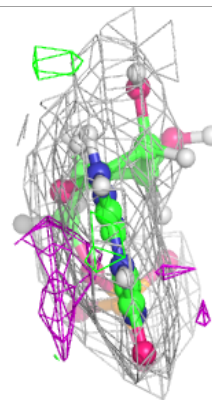
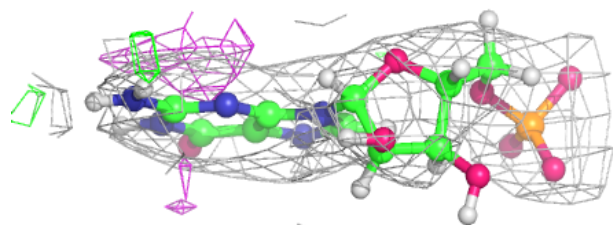
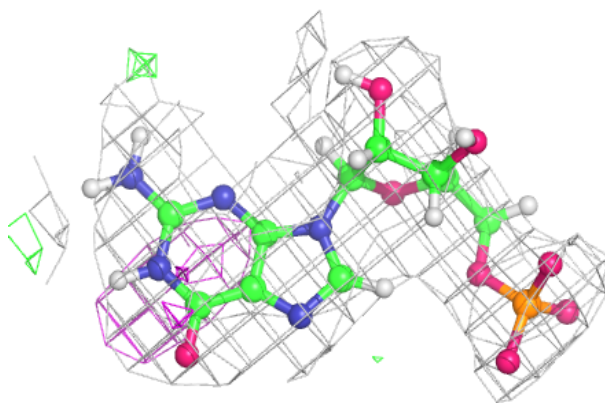
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



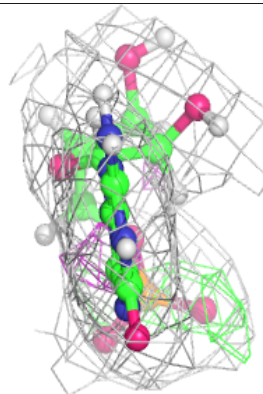
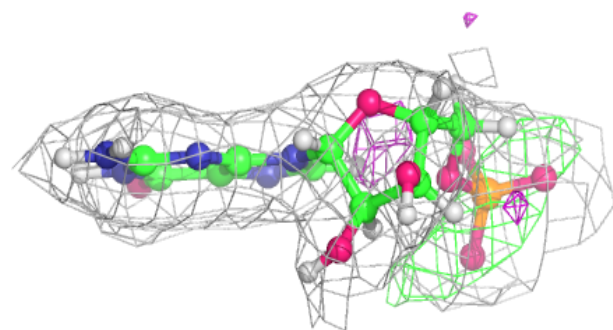
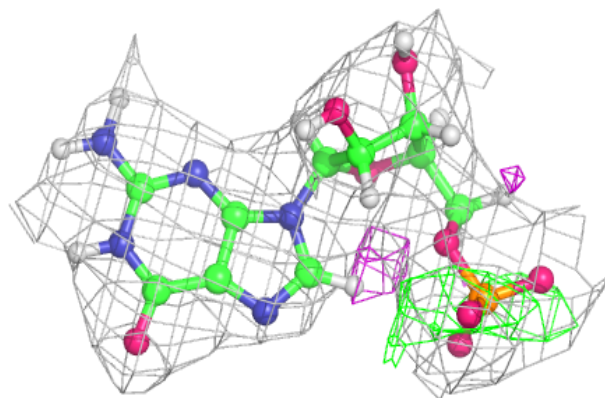


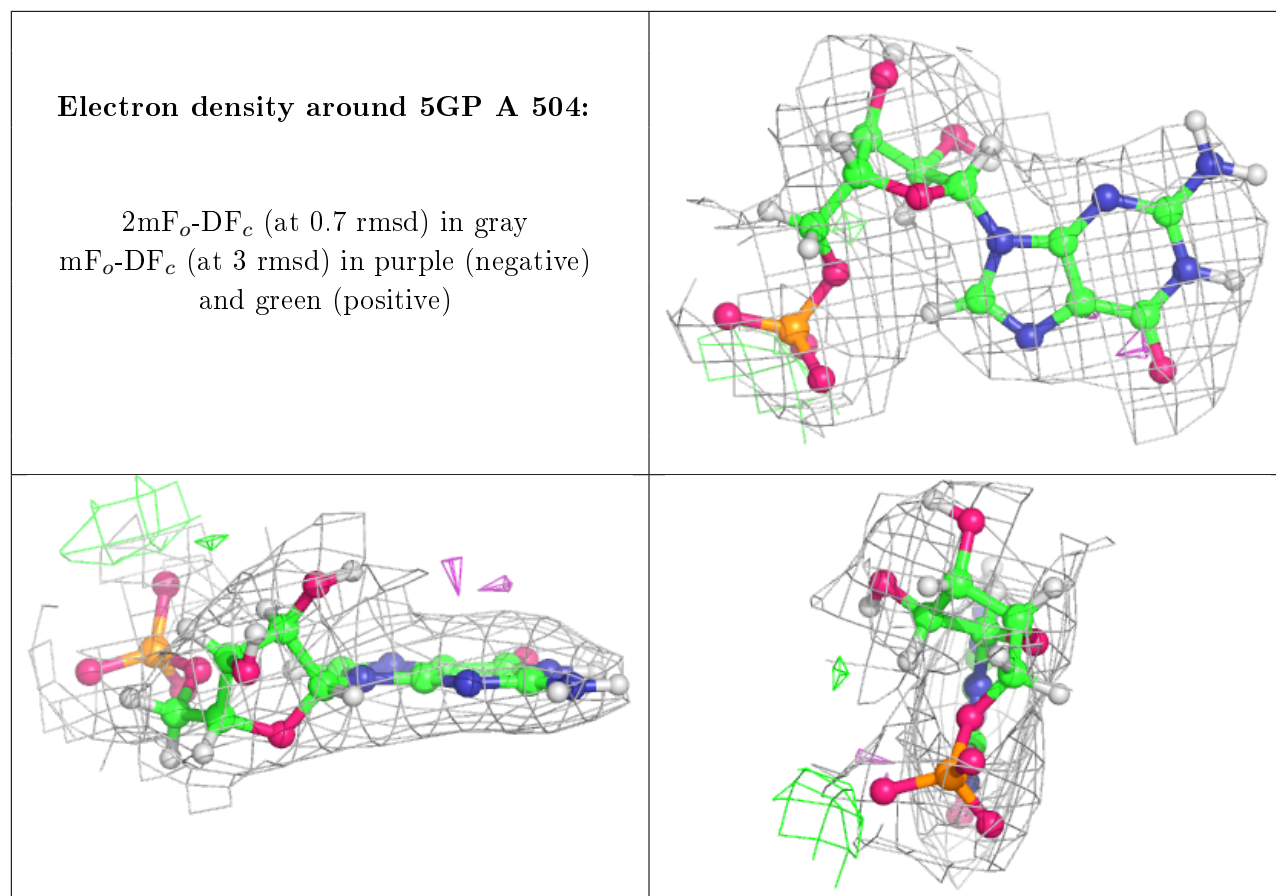
**Electron density around 5GP A 503:**

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

**Electron density around 5GP A 502:**

$2mF_o-DF_c$  (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.