



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:32 am BST

PDB ID : 5FBL  
Title : PI4KB in complex with Rab11 and the MI356 Inhibitor  
Authors : Chalupska, D.; Mejdrova, I.; Nencka, R.; Boura, E.  
Deposited on : 2015-12-14  
Resolution : 3.37 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

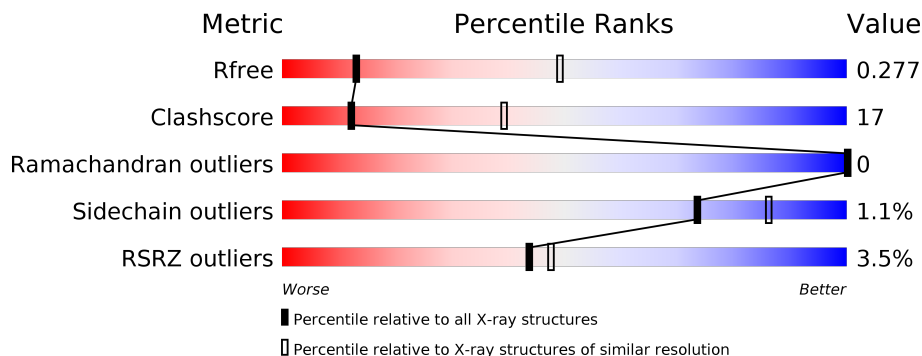
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.37 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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	572	 % 59% 22% 19%
2	B	221	 7% 48% 25% 27%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5031 atoms, of which 14 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 4-kinase beta, Phosphatidylinositol 4-kinase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	465	3749	2409	648	668	24	0	0	0

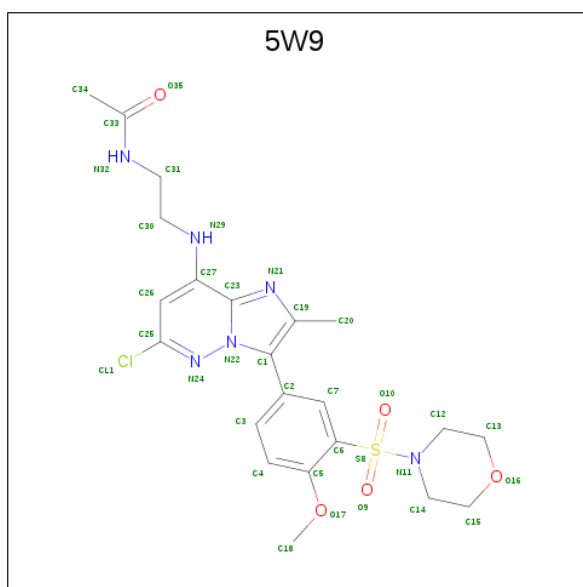
- Molecule 2 is a protein called Ras-related protein Rab-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	162	1201	759	203	238	1	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

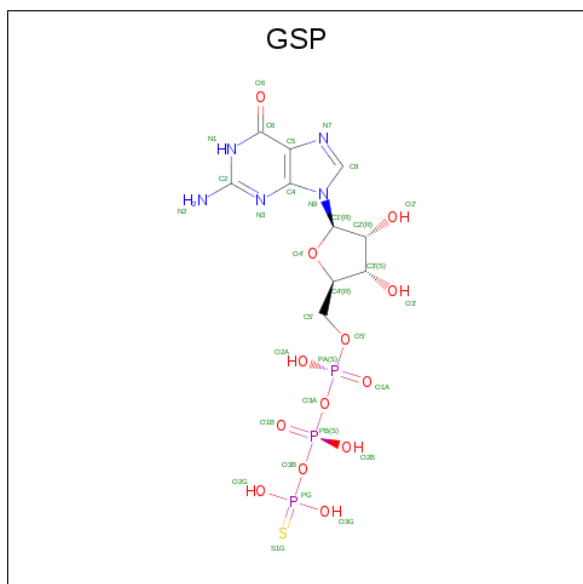
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P62491
B	-3	ALA	-	expression tag	UNP P62491
B	-2	MET	-	expression tag	UNP P62491
B	-1	GLY	-	expression tag	UNP P62491
B	0	SER	-	expression tag	UNP P62491

- Molecule 3 is {N}-[2-[[6-chloranyl-3-(4-methoxy-3-morpholin-4-ylsulfonyl-phenyl)-2-methyl-imidazo[1,2-b]pyridazin-8-yl]amino]ethyl]ethanamide (three-letter code: 5W9) (formula: C<sub>22</sub>H<sub>27</sub>ClN<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
3	A	1	35	22	1	6	5	1	0	0

- Molecule 4 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
			Total	C	H	N	O	P			S
4	B	1	46	10	14	5	13	3	1	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.48Å 104.90Å 188.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.01 – 3.37 47.01 – 3.37	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.01-3.37) 92.2 (47.01-3.37)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 3.40Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.243 , 0.269 0.247 , 0.277	Depositor DCC
$R_{free}$ test set	720 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.0	Xtrriage
Anisotropy	0.879	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 76.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: GSP, 5W9

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	0.25	0/3826	0.47	1/5165 (0.0%)
2	B	0.26	0/1216	0.61	0/1655
All	All	0.26	0/5042	0.51	1/6820 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	348	LEU	C-N-CD	5.76	140.50	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	47	GLU	Peptide

### 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	3749	0	3801	117	0
2	B	1201	0	1150	57	0
3	A	35	0	0	1	0
4	B	32	14	11	3	0
All	All	5017	14	4962	170	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 17.

All (170) 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:351:ARG:HB3	1:A:399:VAL:CG1	1.67	1.23
1:A:351:ARG:HA	1:A:362:HIS:CD2	1.82	1.15
1:A:351:ARG:HB3	1:A:399:VAL:HG11	1.15	1.09
1:A:351:ARG:HA	1:A:362:HIS:HD2	1.00	1.07
2:B:65:TRP:O	2:B:80:TYR:OH	1.81	0.99
1:A:351:ARG:CB	1:A:399:VAL:CG1	2.45	0.93
2:B:88:LEU:HD23	2:B:120:MET:HB3	1.50	0.92
1:A:351:ARG:CB	1:A:399:VAL:HG12	2.09	0.83
1:A:351:ARG:HB3	1:A:399:VAL:HG12	1.59	0.82
2:B:28:LEU:HD11	2:B:49:ALA:HB3	1.60	0.81
1:A:355:PRO:HG2	1:A:601:LEU:HD22	1.64	0.79
1:A:628:LEU:HD22	1:A:632:ASP:HB3	1.68	0.74
1:A:643:THR:HG23	1:A:646:PHE:H	1.53	0.74
2:B:55:VAL:HG22	2:B:60:ILE:HD13	1.68	0.74
2:B:172:ILE:O	2:B:175:ILE:HG13	1.89	0.73
1:A:564:LYS:NZ	3:A:801:5W9:O9	2.22	0.72
1:A:379:LYS:HD2	1:A:566:GLY:HA3	1.71	0.71
1:A:672:ARG:NH2	1:A:689:ASP:O	2.24	0.71
1:A:206:ILE:HD11	1:A:394:PHE:CE2	2.26	0.70
1:A:351:ARG:CA	1:A:362:HIS:HD2	1.93	0.70
1:A:329:THR:HG23	1:A:332:GLN:H	1.56	0.70
1:A:641:TYR:HA	1:A:646:PHE:CD2	2.27	0.69
1:A:356:THR:HG21	1:A:561:VAL:HG12	1.74	0.68
2:B:121:LEU:HB2	2:B:148:LEU:HD13	1.76	0.68
2:B:25:SER:OG	4:B:301:GSP:S1G	2.52	0.68
2:B:106:LEU:O	2:B:110:ARG:HG3	1.93	0.67
2:B:94:ALA:HB1	2:B:131:LEU:HD22	1.75	0.66
2:B:16:LEU:CD2	2:B:88:LEU:HB2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:VAL:HG23	1:A:622:VAL:HG23	1.78	0.65
2:B:143:ALA:HA	2:B:148:LEU:HD11	1.77	0.65
1:A:652:ASN:HB3	1:A:684:HIS:CD2	2.33	0.64
2:B:26:ASN:ND2	4:B:301:GSP:O1A	2.32	0.64
1:A:544:ILE:HD12	1:A:558:LEU:HD21	1.80	0.63
1:A:640:SER:O	1:A:643:THR:HG22	1.98	0.63
1:A:631:LEU:HA	1:A:717:VAL:HG22	1.80	0.63
1:A:134:PHE:O	1:A:163:ARG:NH1	2.32	0.62
1:A:141:ILE:HD13	1:A:172:VAL:HG22	1.81	0.62
1:A:149:TYR:HB2	1:A:182:MET:CE	2.29	0.62
1:A:351:ARG:O	1:A:351:ARG:HG3	1.99	0.62
1:A:593:LEU:HD21	1:A:732:LEU:HB3	1.80	0.62
1:A:324:LEU:O	1:A:333:LYS:HE3	2.00	0.61
2:B:9:ASP:HB2	2:B:59:THR:O	2.00	0.61
2:B:17:ILE:HD12	2:B:105:TRP:CE3	2.36	0.60
2:B:94:ALA:HB1	2:B:131:LEU:CD2	2.31	0.60
1:A:744:MET:CE	1:A:773:LYS:HA	2.31	0.60
1:A:131:LEU:HD22	2:B:36:PHE:CE2	2.37	0.60
1:A:351:ARG:CB	1:A:399:VAL:HG11	2.09	0.59
2:B:13:LYS:HD3	2:B:63:GLN:HB3	1.84	0.59
1:A:751:VAL:HG12	1:A:769:ILE:HD11	1.84	0.59
1:A:165:PHE:CZ	1:A:197:TYR:HA	2.37	0.59
2:B:32:THR:HG21	2:B:49:ALA:HB1	1.83	0.59
1:A:195:LYS:HB3	1:A:196:PRO:HD3	1.85	0.58
1:A:329:THR:HG22	1:A:332:GLN:HB2	1.84	0.58
1:A:130:LEU:HB2	2:B:39:GLU:OE2	2.03	0.58
1:A:598:TYR:OH	1:A:688:ILE:O	2.21	0.57
1:A:356:THR:HG21	1:A:561:VAL:CG1	2.35	0.57
2:B:16:LEU:HD23	2:B:88:LEU:HB2	1.85	0.57
1:A:310:GLU:OE1	1:A:352:VAL:HB	2.06	0.56
1:A:318:MET:HE1	1:A:563:VAL:HG13	1.87	0.56
1:A:354:LEU:HD13	1:A:561:VAL:CG1	2.36	0.55
1:A:149:TYR:HB2	1:A:182:MET:HE2	1.89	0.55
1:A:751:VAL:HG12	1:A:769:ILE:CD1	2.36	0.55
2:B:54:GLN:HG3	2:B:59:THR:HA	1.89	0.55
1:A:130:LEU:HD22	2:B:39:GLU:HG3	1.88	0.55
1:A:354:LEU:H	1:A:361:HIS:CE1	2.25	0.55
2:B:13:LYS:HB3	2:B:83:GLY:O	2.07	0.54
1:A:139:PHE:HA	1:A:143:MET:HE2	1.89	0.54
1:A:343:LEU:O	1:A:346:HIS:HB2	2.08	0.54
1:A:619:ILE:O	1:A:623:LYS:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:LEU:CD2	2:B:120:MET:HB3	2.32	0.54
1:A:206:ILE:HD11	1:A:394:PHE:CD2	2.42	0.54
2:B:118:VAL:HG21	2:B:172:ILE:HD13	1.90	0.54
1:A:617:VAL:HG23	1:A:622:VAL:CG2	2.38	0.53
2:B:13:LYS:CG	2:B:83:GLY:O	2.56	0.53
2:B:128:LEU:HD21	4:B:301:GSP:N2	2.24	0.53
2:B:131:LEU:O	2:B:131:LEU:HD23	2.07	0.53
1:A:581:GLN:HE22	1:A:746:LYS:HD3	1.74	0.52
2:B:79:ALA:O	2:B:82:ARG:HB3	2.08	0.52
1:A:564:LYS:HE3	1:A:567:ASP:HB2	1.92	0.52
1:A:568:ASP:C	1:A:569:LEU:HD23	2.30	0.51
2:B:15:VAL:HB	2:B:80:TYR:CE1	2.44	0.51
2:B:53:ILE:HD11	2:B:169:LEU:HD12	1.92	0.51
1:A:403:ILE:HG22	1:A:549:PRO:HB3	1.93	0.51
1:A:781:THR:HG22	1:A:784:GLN:CG	2.41	0.51
2:B:136:THR:HG22	2:B:140:ARG:HH12	1.76	0.51
1:A:533:LEU:HG	1:A:534:LYS:H	1.75	0.51
1:A:579:LEU:HD21	1:A:663:VAL:HG11	1.93	0.51
1:A:355:PRO:HG2	1:A:601:LEU:CD2	2.39	0.50
1:A:323:ARG:NH2	1:A:340:GLU:OE2	2.41	0.50
2:B:53:ILE:CD1	2:B:169:LEU:HD12	2.42	0.49
1:A:715:VAL:HG11	1:A:721:LEU:CD2	2.42	0.49
1:A:715:VAL:HG11	1:A:721:LEU:HD23	1.94	0.49
1:A:318:MET:CE	1:A:563:VAL:HG13	2.42	0.49
1:A:139:PHE:HD1	1:A:143:MET:HE2	1.78	0.49
1:A:182:MET:HA	1:A:186:MET:HG3	1.94	0.48
1:A:340:GLU:HG3	1:A:343:LEU:HD12	1.95	0.48
1:A:351:ARG:HB2	1:A:399:VAL:HG12	1.95	0.48
2:B:60:ILE:HG22	2:B:61:LYS:N	2.27	0.48
1:A:354:LEU:HD13	1:A:561:VAL:HG13	1.95	0.48
1:A:329:THR:HG22	1:A:332:GLN:CG	2.44	0.48
2:B:16:LEU:HD21	2:B:88:LEU:HD12	1.95	0.48
1:A:568:ASP:O	1:A:569:LEU:HD23	2.14	0.47
2:B:165:PHE:O	2:B:168:ILE:HG22	2.13	0.47
1:A:544:ILE:HD12	1:A:558:LEU:CD2	2.45	0.47
1:A:767:SER:HB3	1:A:770:ARG:HB2	1.95	0.47
1:A:593:LEU:CD2	1:A:732:LEU:HB3	2.43	0.47
1:A:541:VAL:O	1:A:545:ARG:HB2	2.14	0.47
1:A:389:LEU:HD22	1:A:555:ASN:HB3	1.96	0.47
1:A:749:GLN:O	1:A:753:ILE:HG13	2.15	0.47
1:A:362:HIS:CD2	1:A:399:VAL:HG12	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LEU:HG	1:A:534:LYS:N	2.29	0.47
1:A:206:ILE:HD11	1:A:394:PHE:HE2	1.73	0.47
1:A:341:LEU:O	1:A:344:LEU:HB2	2.15	0.47
1:A:178:GLN:HA	1:A:754:MET:HE2	1.96	0.46
1:A:236:LEU:O	1:A:240:ILE:HG13	2.15	0.46
1:A:781:THR:HG22	1:A:784:GLN:HG3	1.98	0.46
2:B:121:LEU:CB	2:B:148:LEU:HD13	2.44	0.46
1:A:581:GLN:NE2	1:A:746:LYS:HD3	2.31	0.46
2:B:58:LYS:O	2:B:60:ILE:HD12	2.15	0.46
1:A:783:GLU:CD	1:A:783:GLU:H	2.20	0.46
2:B:60:ILE:CG2	2:B:61:LYS:N	2.78	0.46
1:A:631:LEU:HD13	1:A:717:VAL:HA	1.97	0.45
2:B:89:LEU:CD2	2:B:102:VAL:HG13	2.45	0.45
1:A:576:PHE:CZ	1:A:580:LYS:HD3	2.52	0.45
1:A:393:ASN:HB3	1:A:396:THR:HG22	1.99	0.45
1:A:354:LEU:HD13	1:A:561:VAL:HG11	1.99	0.45
1:A:344:LEU:HA	1:A:344:LEU:HD23	1.85	0.45
1:A:633:TYR:CZ	1:A:637:GLU:HG3	2.53	0.44
1:A:131:LEU:HD22	2:B:36:PHE:HE2	1.81	0.44
2:B:139:ALA:HB1	2:B:150:PHE:CE1	2.52	0.44
2:B:30:ARG:O	2:B:34:ASN:HA	2.17	0.44
2:B:136:THR:HG22	2:B:140:ARG:NH1	2.32	0.44
2:B:109:LEU:C	2:B:109:LEU:HD23	2.37	0.44
1:A:176:LEU:N	1:A:177:PRO:CD	2.81	0.44
1:A:329:THR:HG22	1:A:332:GLN:CB	2.48	0.44
1:A:405:GLU:HA	1:A:405:GLU:OE1	2.18	0.44
1:A:781:THR:HG23	1:A:784:GLN:H	1.82	0.44
2:B:136:THR:CG2	2:B:140:ARG:HH12	2.30	0.44
1:A:344:LEU:O	1:A:347:LYS:HB3	2.18	0.44
2:B:16:LEU:O	2:B:80:TYR:OH	2.36	0.44
1:A:798:ARG:O	1:A:799:SER:CB	2.66	0.44
1:A:755:GLN:HB2	1:A:763:PHE:CD1	2.53	0.43
2:B:15:VAL:HB	2:B:80:TYR:HE1	1.83	0.43
2:B:143:ALA:HB1	2:B:150:PHE:HB2	2.01	0.43
2:B:148:LEU:O	2:B:148:LEU:HD12	2.19	0.43
1:A:368:HIS:CE1	1:A:369:THR:HG23	2.54	0.43
1:A:329:THR:CG2	1:A:332:GLN:HG3	2.49	0.42
1:A:657:CYS:HB3	1:A:729:TYR:CE1	2.54	0.42
1:A:177:PRO:HB2	1:A:754:MET:CE	2.49	0.42
2:B:60:ILE:N	2:B:60:ILE:HD12	2.35	0.42
1:A:214:LEU:HD22	1:A:603:ILE:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:ARG:HA	2:B:143:ALA:HB3	2.00	0.42
1:A:544:ILE:CD1	1:A:558:LEU:HD21	2.49	0.42
1:A:755:GLN:HB2	1:A:763:PHE:CE1	2.55	0.42
2:B:143:ALA:CA	2:B:148:LEU:HD11	2.48	0.42
1:A:405:GLU:OE1	1:A:549:PRO:HG3	2.20	0.41
2:B:11:LEU:O	2:B:11:LEU:HD23	2.20	0.41
2:B:87:ALA:O	2:B:119:ILE:HA	2.20	0.41
1:A:308:ALA:HB3	1:A:309:PRO:HD3	2.02	0.41
1:A:351:ARG:CA	1:A:362:HIS:CD2	2.76	0.41
2:B:13:LYS:CB	2:B:83:GLY:O	2.69	0.41
1:A:769:ILE:O	1:A:773:LYS:HG3	2.21	0.41
1:A:307:LEU:O	1:A:311:ARG:HG3	2.21	0.41
1:A:619:ILE:HD11	1:A:679:LEU:HB2	2.02	0.41
1:A:379:LYS:HB2	1:A:379:LYS:HE3	1.72	0.40
1:A:389:LEU:HD23	1:A:556:TRP:HA	2.03	0.40
1:A:540:LYS:O	1:A:544:ILE:HG13	2.21	0.40
1:A:755:GLN:O	1:A:755:GLN:HG2	2.21	0.40
1:A:695:SER:CB	1:A:765:GLY:H	2.35	0.40
2:B:93:ILE:C	2:B:93:ILE:HD12	2.42	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	455/572 (80%)	443 (97%)	12 (3%)	0	100	100
2	B	158/221 (72%)	148 (94%)	10 (6%)	0	100	100
All	All	613/793 (77%)	591 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

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

In the following table, the Percentiles column shows the percent 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	416/517 (80%)	412 (99%)	4 (1%)	76	87
2	B	122/191 (64%)	120 (98%)	2 (2%)	62	81
All	All	538/708 (76%)	532 (99%)	6 (1%)	73	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	LEU
1	A	351	ARG
1	A	391	CYS
1	A	405	GLU
2	B	46	VAL
2	B	80	TYR

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	362	HIS
1	A	581	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 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
4	GSP	B	301	-	26,34,34	4.30	13 (50%)	28,54,54	2.70	8 (28%)
3	5W9	A	801	-	34,38,38	2.88	6 (17%)	42,55,55	2.36	15 (35%)

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
4	GSP	B	301	-	-	7/17/38/38	0/3/3/3
3	5W9	A	801	-	-	8/25/33/33	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	5W9	C6-S8	-13.63	1.60	1.78
4	B	301	GSP	C2'-C3'	-10.88	1.23	1.53
4	B	301	GSP	O4'-C1'	7.74	1.51	1.41
4	B	301	GSP	O4'-C4'	-7.15	1.29	1.45
4	B	301	GSP	C6-C5	6.99	1.53	1.41
4	B	301	GSP	C4-N3	6.91	1.46	1.35
3	A	801	5W9	C1-C19	6.65	1.48	1.37
4	B	301	GSP	C3'-C4'	5.68	1.67	1.53
4	B	301	GSP	C2-N2	5.11	1.44	1.33
4	B	301	GSP	C6-N1	4.88	1.41	1.33
4	B	301	GSP	C2-N1	4.43	1.43	1.35
3	A	801	5W9	C27-C23	3.88	1.49	1.42
4	B	301	GSP	C2'-C1'	3.85	1.59	1.53
4	B	301	GSP	O2'-C2'	3.66	1.51	1.43
3	A	801	5W9	C23-N21	3.50	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	5W9	C25-N24	3.02	1.35	1.31
4	B	301	GSP	C2-N3	2.82	1.47	1.34
3	A	801	5W9	C25-CL1	2.71	1.80	1.74
4	B	301	GSP	PG-S1G	2.28	1.95	1.90

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	GSP	C1'-N9-C4	10.32	144.77	126.64
3	A	801	5W9	O9-S8-O10	-6.63	108.78	119.52
3	A	801	5W9	O17-C5-C6	6.49	121.53	116.50
4	B	301	GSP	N3-C2-N1	-5.23	120.24	127.22
3	A	801	5W9	CL1-C25-N24	4.33	119.63	115.19
3	A	801	5W9	C12-N11-S8	-3.95	109.86	117.05
3	A	801	5W9	C14-N11-S8	-3.93	109.91	117.05
4	B	301	GSP	C2-N3-C4	3.75	119.64	115.36
3	A	801	5W9	O17-C5-C4	-3.37	118.60	124.37
4	B	301	GSP	C2'-C3'-C4'	3.29	109.04	102.64
3	A	801	5W9	O9-S8-N11	3.28	109.68	106.69
3	A	801	5W9	C19-N21-C23	3.07	109.00	103.59
4	B	301	GSP	C3'-C2'-C1'	2.94	105.41	100.98
3	A	801	5W9	C26-C25-N24	-2.92	120.74	125.03
4	B	301	GSP	PA-O3A-PB	-2.49	124.27	132.83
3	A	801	5W9	C15-C14-N11	2.47	109.63	108.18
4	B	301	GSP	C5-C6-N1	-2.43	120.11	123.43
3	A	801	5W9	C2-C1-N22	-2.35	119.94	123.37
3	A	801	5W9	C14-N11-C12	-2.31	109.61	112.17
3	A	801	5W9	C25-C26-C27	2.30	120.28	116.85
4	B	301	GSP	C6-N1-C2	2.21	119.44	115.93
3	A	801	5W9	C13-C12-N11	2.17	109.45	108.18
3	A	801	5W9	O10-S8-N11	2.10	108.61	106.69

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	GSP	PB-O3B-PG-O3G
4	B	301	GSP	C5'-O5'-PA-O3A
3	A	801	5W9	C34-C33-N32-C31
3	A	801	5W9	C30-C31-N32-C33
4	B	301	GSP	O4'-C4'-C5'-O5'
3	A	801	5W9	C4-C5-O17-C18

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Mol	Chain	Res	Type	Atoms
3	A	801	5W9	C6-C5-O17-C18
3	A	801	5W9	O35-C33-N32-C31
4	B	301	GSP	C3'-C4'-C5'-O5'
3	A	801	5W9	C14-N11-S8-O10
4	B	301	GSP	PB-O3A-PA-O2A
4	B	301	GSP	C5'-O5'-PA-O1A
4	B	301	GSP	C5'-O5'-PA-O2A
3	A	801	5W9	C5-C6-S8-O10
3	A	801	5W9	C5-C6-S8-O9

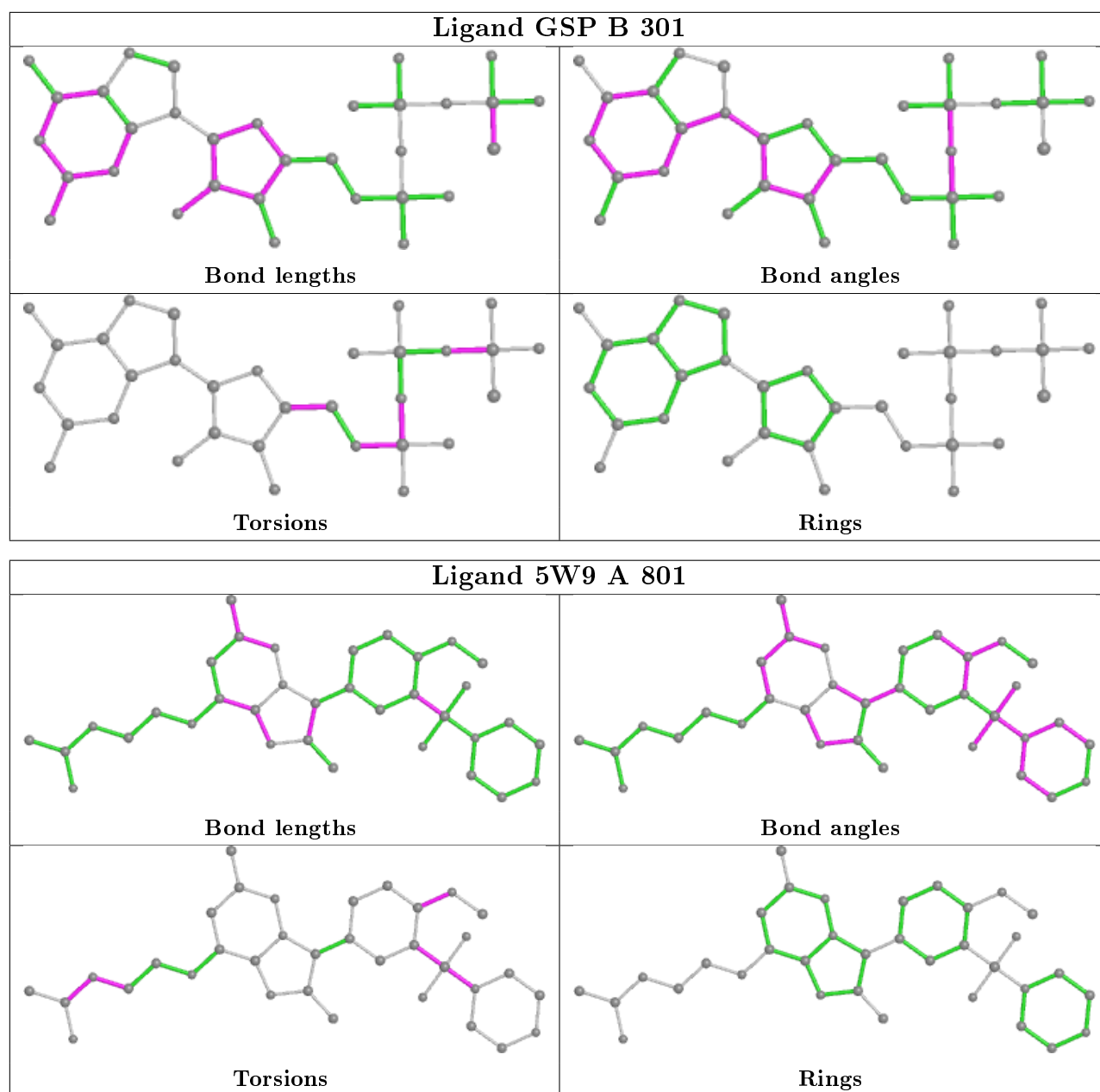
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	GSP	3	0
3	A	801	5W9	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	465/572 (81%)	0.19	7 (1%) 73 77	78, 111, 142, 163	0
2	B	162/221 (73%)	0.63	15 (9%) 8 11	105, 139, 156, 165	0
All	All	627/793 (79%)	0.30	22 (3%) 44 47	78, 118, 152, 165	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	62	ALA	5.8
2	B	12	PHE	5.4
1	A	799	SER	4.7
2	B	55	VAL	4.7
2	B	53	ILE	3.6
2	B	60	ILE	3.4
2	B	39	GLU	3.1
1	A	641	TYR	2.9
2	B	99	TYR	2.9
2	B	38	LEU	2.5
2	B	119	ILE	2.5
1	A	339	SER	2.5
1	A	234	THR	2.5
2	B	52	SER	2.4
2	B	51	ARG	2.4
2	B	89	LEU	2.4
1	A	139	PHE	2.3
2	B	64	ILE	2.2
2	B	118	VAL	2.2
1	A	219	TYR	2.1
1	A	531	VAL	2.1
2	B	120	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](#)

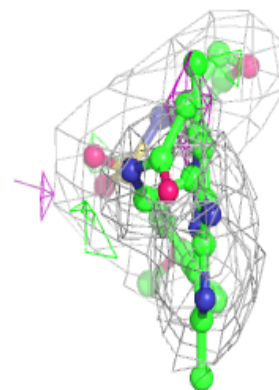
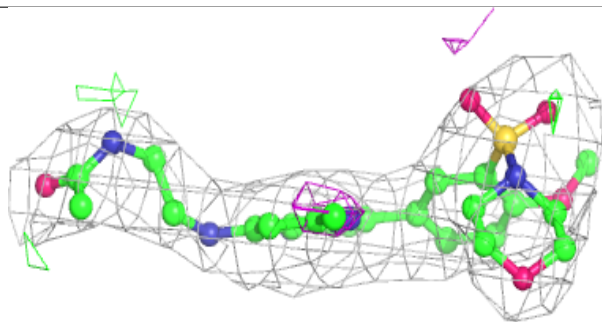
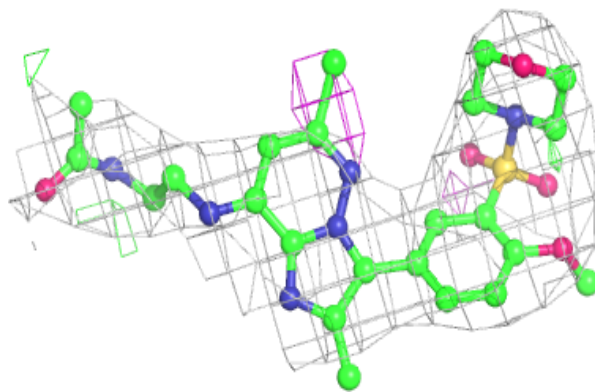
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	5W9	A	801	35/35	0.89	0.29	91,109,136,279	0
4	GSP	B	301	32/32	0.91	0.17	109,123,147,168	0

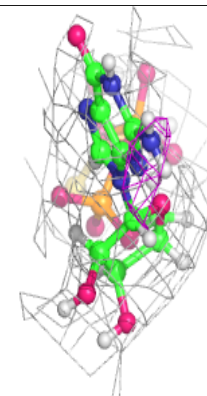
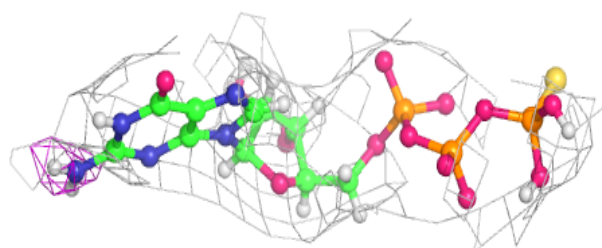
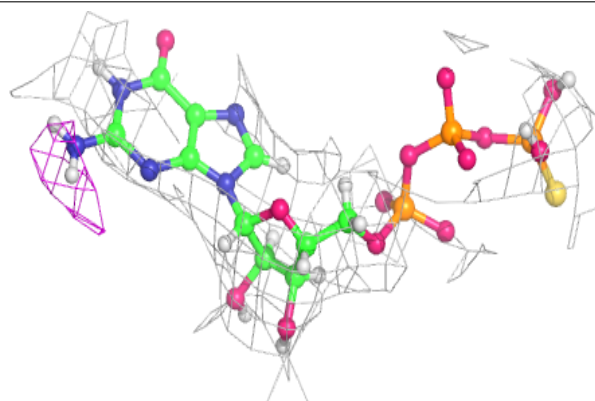
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 5W9 A 801:**

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

**Electron density around GSP B 301:**

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



## 6.5 Other polymers

There are no such residues in this entry.