



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:44 PM GMT

PDB ID : 3X06  
Title : Crystal structure of PIP4KIIBETA T201M complex with GMP  
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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  
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

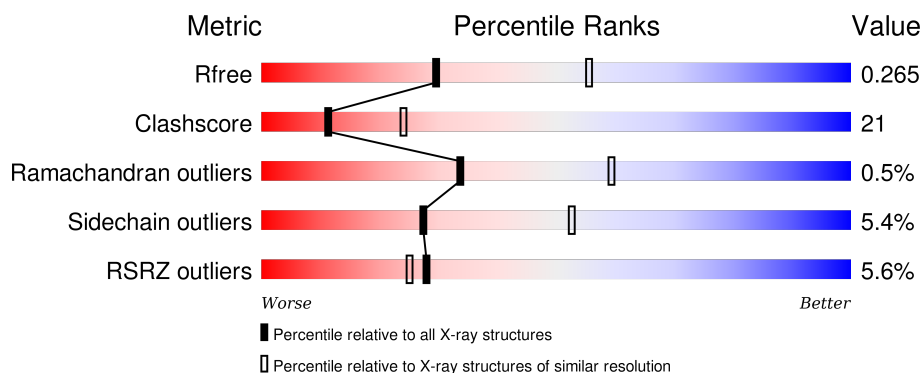
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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. 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	<div> <div>2%</div> <div>53%</div> <div>26%</div> <div>•</div> <div>19%</div> </div>
1	B	393	<div> <div>7%</div> <div>50%</div> <div>24%</div> <div>•</div> <div>23%</div> </div>

## 2 Entry composition

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.

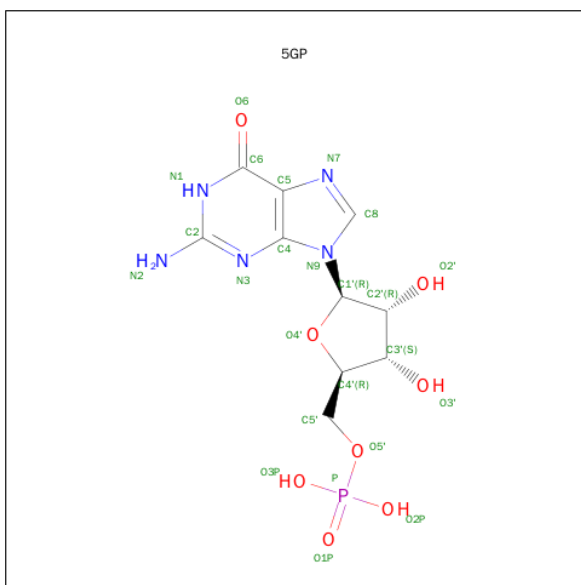
- Molecule 1 is a protein called Phosphatidylinositol 5-phosphate 4-kinase type-2 beta.

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

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
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		



LYS	THR	VAL	LYS	HIS	GLY	ALA	GLY	ALA	GLU	ILE	SER	THR	VAL	ASN	P400	R406	F407	N408	E409	F410	M411	S412	N413	I414	L415	THR
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## 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 0.216 , 0.265	Depositor DCC
$R_{free}$ test set	1548 reflections (5.26%)	DCC
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 , 73.7	EDS
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
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 30965 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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

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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:B:213:ARG:HG2	1:B:215:TYR:CE1	2.23	0.71
1:A:256:SER:HB3	1:A:351:MET:HE1	1.71	0.71

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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:141:THR:HG23	1:B:145:ARG:HA	1.75	0.68
1:B:43:LEU:HD21	1:B:140:LEU:HD11	1.76	0.68
1:B:94:LYS:HB2	1:B:190:THR:HB	1.76	0.67
1:A:218:LYS:HD2	1:A:224:ARG:NE	2.08	0.67
1:A:256:SER:HB3	1:A:351:MET:CE	2.24	0.67
1:B:216:ASP:C	1:B:217:LEU:HD23	2.16	0.66
1:A:42:ILE:H	1:A:42:ILE:HD13	1.60	0.66
1:A:42:ILE:N	1:A:42:ILE:HD13	2.10	0.66
1:B:243:PHE:CE2	1:B:414:ILE:HG22	2.22	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: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

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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:79:VAL:O	1:B:92:ARG:HA	2.01	0.60
1:B:60:VAL:O	1:B:104:ARG:NH2	2.34	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:OD1	1:B:240:ASP:N	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:B:225:GLU:HA	1:B:242:ASP:OD1	2.07	0.55
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: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:264:LEU:HD11	1:A:407:PHE:HE1	1.73	0.54
1:A:236:PRO:HB2	1:A:238:PHE:CE2	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:LYS:CG	1:B:236:PRO:O	2.57	0.52
1:B:141:THR:CG2	1:B:142:THR:O	2.54	0.52
1:B:48:TRP:HH2	1:B:77:ILE:HD13	1.75	0.52
1:B:213:ARG:HG2	1:B:215:TYR:CZ	2.44	0.52
1:B:206:SER:CB	1:B:209:LEU:HB2	2.40	0.52
1:A:217:LEU:CD1	1:A:414:ILE:HD13	2.38	0.51
1:A:139:PHE:CZ	1:A:148:VAL:CG1	2.93	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:HG3	1:B:215:TYR:CZ	2.44	0.51
1:B:213:ARG:HB3	1:B:215:TYR:HE1	1.75	0.51
1:B:407:PHE:C	1:B:407:PHE:CD1	2.84	0.51
1:B:189:LEU:CD1	1:B:189:LEU:N	2.73	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:B:288:VAL:HG23	1:B:360:LYS:O	2.14	0.47
1:A:230:GLU:OE1	1:A:233:LYS:HD2	2.13	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:220:SER:HB2	1:B:406:ARG:HD3	1.97	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:110:PHE:CZ	1:B:182:GLN:HG2	2.49	0.46

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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: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:159:GLU:OE2	1:A:159:GLU:HA	2.16	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:B:264:LEU:O	1:B:268:VAL:HG22	2.17	0.44
1:A:295:GLU:O	1:A:298:VAL:HG12	2.17	0.44
1:B:237:THR:HG22	1:B:237:THR:O	2.17	0.44
1:A:415:LEU:O	1:A:416:THR:CG2	2.66	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:B:276:ILE:HG22	1:B:277:MET:N	2.33	0.43
1:A:287:ASP:HB3	1:A:290:ARG:HB3	1.99	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:B:215:TYR:HB3	1:B:217:LEU:HD21	2.00	0.42
1:A:230:GLU:CD	1:A:233:LYS:HD2	2.40	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:407:PHE:O	1:A:411:MET:HG2	2.20	0.41
1:A:272:ALA:O	1:A:274:LEU:O	2.38	0.41
1:B:40:GLU:HA	1:B:41:PRO:HD3	1.89	0.41
1:B:240:ASP:HB3	1:B:410:PHE:CZ	2.55	0.41
1:A:210:THR:O	1:A:286:HIS:ND1	2.45	0.41
1:A:341:GLU:CG	1:A:342:PHE:N	2.83	0.41

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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:B:213:ARG:HB2	1:B:285:ILE:HB	2.02	0.41
1:B:240:ASP:HB3	1:B:410:PHE:CE2	2.56	0.41
1:A:234:ASP:O	1:A:236:PRO:HD3	2.21	0.41
1:A:274:LEU:HB2	1:A:276:ILE:HG12	2.03	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: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:B:361:GLU:HG3	1:B:363:TYR:CZ	2.56	0.40
1:A:60:VAL:HA	1:A:61:PRO:HD2	1.86	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 ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	310/393 (79%)	297 (96%)	11 (4%)	2 (1%)	30	54
1	B	293/393 (75%)	283 (97%)	9 (3%)	1 (0%)	46	72
All	All	603/786 (77%)	580 (96%)	20 (3%)	3 (0%)	34	59

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 ⓘ

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%)	23	46
1	B	281/352 (80%)	268 (95%)	13 (5%)	33	61
All	All	576/704 (82%)	545 (95%)	31 (5%)	27	52

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

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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 ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	0.96	2 (9%)	22,40,40	0.95	2 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	5GP	A	502	-	22,26,26	2.21	11 (50%)	22,40,40	1.58	4 (18%)
2	5GP	A	503	-	22,26,26	0.88	1 (4%)	22,40,40	1.08	3 (13%)
2	5GP	A	504	-	22,26,26	1.06	2 (9%)	22,40,40	0.99	3 (13%)
2	5GP	B	501	-	22,26,26	0.92	2 (9%)	22,40,40	0.88	1 (4%)

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	-	-	0/6/26/26	0/3/3/3
2	5GP	A	502	-	-	0/6/26/26	0/3/3/3
2	5GP	A	503	-	-	0/6/26/26	0/3/3/3
2	5GP	A	504	-	-	0/6/26/26	0/3/3/3
2	5GP	B	501	-	-	0/6/26/26	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	5GP	C6-N1	-4.94	1.29	1.36
2	A	502	5GP	C2-N1	-3.90	1.30	1.36
2	A	502	5GP	P-O3P	-2.91	1.44	1.54
2	A	502	5GP	P-O2P	-2.78	1.45	1.54
2	A	501	5GP	C6-N1	-2.46	1.33	1.36
2	A	502	5GP	C2'-C1'	-2.44	1.49	1.53
2	A	502	5GP	O4'-C4'	-2.34	1.39	1.45
2	A	502	5GP	C4-N3	-2.30	1.32	1.35
2	A	502	5GP	P-O5'	-2.29	1.53	1.59
2	A	502	5GP	C2'-C3'	-2.23	1.47	1.53
2	B	501	5GP	C6-N1	-2.22	1.33	1.36
2	A	502	5GP	P-O1P	-2.22	1.43	1.50
2	A	504	5GP	C2-N3	2.19	1.36	1.33
2	B	501	5GP	C2-N2	2.27	1.35	1.32
2	A	502	5GP	C6-C5	2.39	1.45	1.40
2	A	501	5GP	C2-N2	2.42	1.36	1.32
2	A	503	5GP	C2-N2	2.57	1.36	1.32
2	A	504	5GP	C2-N2	2.89	1.36	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	5GP	N2-C2-N3	-3.40	115.92	120.29
2	A	503	5GP	O3P-P-O5'	-2.64	99.03	106.72
2	A	501	5GP	O3P-P-O5'	-2.61	99.10	106.72
2	A	502	5GP	O2P-P-O5'	-2.28	100.06	106.72
2	A	504	5GP	O3P-P-O5'	-2.21	100.27	106.72
2	A	502	5GP	C2'-C1'-N9	-2.14	107.73	113.47
2	A	504	5GP	N2-C2-N1	2.24	120.40	117.82
2	A	503	5GP	O2P-P-O1P	2.29	118.11	110.63
2	B	501	5GP	O2P-P-O1P	2.29	118.11	110.63
2	A	501	5GP	O2P-P-O1P	2.34	118.25	110.63
2	A	504	5GP	O2P-P-O1P	2.37	118.35	110.63
2	A	503	5GP	N2-C2-N1	2.37	120.55	117.82
2	A	502	5GP	O3P-P-O1P	2.89	120.07	110.63

There are no chirality outliers.

There are no torsion outliers.

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

## 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%) 61 59	38, 70, 122, 158	0
1	B	303/393 (77%)	0.84	27 (8%) 12 9	38, 76, 143, 160	0
All	All	621/786 (79%)	0.71	35 (5%) 28 25	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	3.1
1	A	406	ARG	3.0
1	B	235	LEU	2.9
1	B	238	PHE	2.8
1	A	302	ALA	2.7
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	208	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	229	LYS	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	B	277	MET	2.2
1	A	209	LEU	2.2
1	A	33	VAL	2.2
1	B	94	LYS	2.1
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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	5GP	B	501	24/24	0.81	0.28	0.75	97,157,195,203	0
2	5GP	A	501	24/24	0.79	0.26	0.65	72,149,195,202	0
2	5GP	A	503	24/24	0.86	0.22	-0.15	70,111,175,180	0
2	5GP	A	504	24/24	0.94	0.21	-0.50	54,77,95,100	0
2	5GP	A	502	24/24	0.92	0.21	-0.70	65,83,102,118	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.