



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:23 AM GMT

PDB ID : 2WXF  
Title : THE CRYSTAL STRUCTURE OF THE MURINE CLASS IA PI 3-KINASE P110DELTA IN COMPLEX WITH PIK-39.  
Authors : Berndt, A.; Miller, S.; Williams, O.; Lee, D.D.; Houseman, B.T.; Pacold, J.I.; Gorrec, F.; Hon, W.-C.; Liu, Y.; Rommel, C.; Gaillard, P.; Ruckle, T.; Schwarz, M.K.; Shokat, K.M.; Shaw, J.P.; Williams, R.L.  
Deposited on : 2009-11-09  
Resolution : 1.90 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

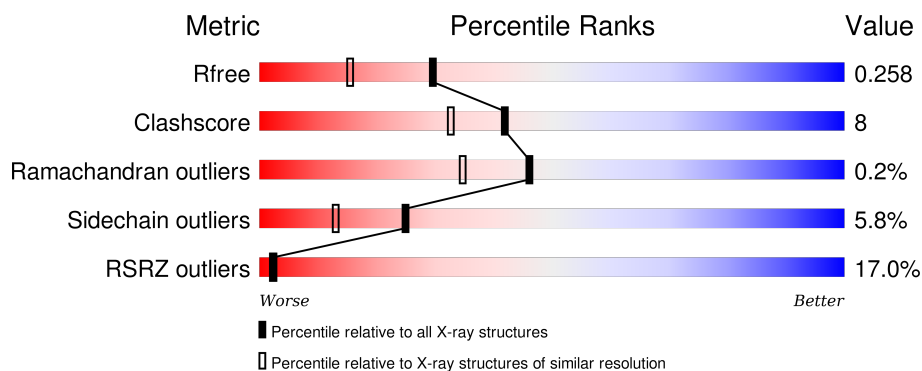
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	940	<div> <div>15%</div> <div>73%</div> <div>13%</div> <div>•</div> <div>13%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6940 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.

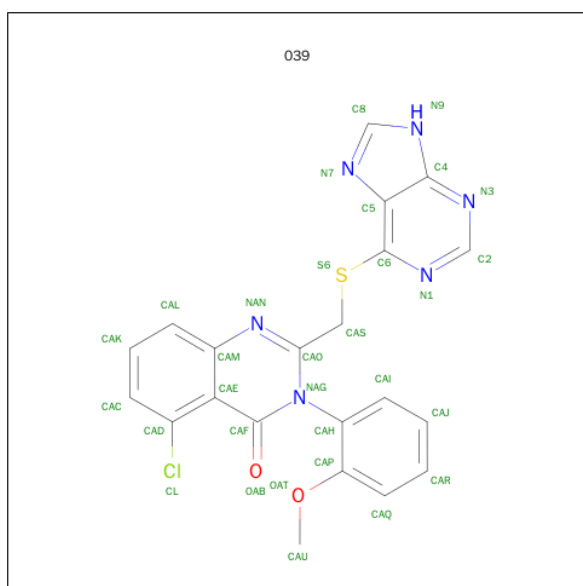
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	5	0
			6667	4273	1132	1206	56			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	-	EXPRESSION TAG	UNP Q3UDT3

- Molecule 2 is 2-((9H-PURIN-6-YLTHIO)METHYL)-5-CHLORO-3-(2-METHOXYPHENYL)QUINAZOLIN-4(3H)-ONE (three-letter code: 039) (formula: C<sub>21</sub>H<sub>15</sub>ClN<sub>6</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			31	21	1	6	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	242	Total 242	O 242	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.42Å 65.01Å 116.69Å 90.00° 103.53° 90.00°	Depositor
Resolution (Å)	38.95 – 1.90 38.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.95-1.90) 98.4 (38.95-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, $R_{free}$	0.210 , 0.240 0.230 , 0.258	Depositor DCC
$R_{free}$ test set	2436 reflections (3.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 80510 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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:  
039

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	0.59	1/6810 (0.0%)	0.63	5/9188 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	ALA	C-O	13.40	1.48	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	902	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	A	902	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	714	MET	CG-SD-CE	-6.36	90.02	100.20
1	A	423	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	634	LEU	CB-CG-CD1	5.13	119.73	111.00

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	6667	0	6642	112	1
2	A	31	0	15	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	242	0	0	13	0
All	All	6940	0	6657	112	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 8.

All (112) 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:899:ILE:CG2	1:A:907[B]:LEU:HD11	1.48	1.41
1:A:367:SER:HB3	1:A:368:GLU:C	1.51	1.29
1:A:367:SER:HB3	1:A:369:PRO:N	1.52	1.24
1:A:899:ILE:HG21	1:A:907[B]:LEU:HD11	1.36	1.07
1:A:899:ILE:HG22	1:A:907[B]:LEU:HD11	1.39	1.02
1:A:899:ILE:CG2	1:A:907[B]:LEU:CD1	2.38	1.02
1:A:795:GLN:HG2	3:A:2151:HOH:O	1.59	1.01
1:A:367:SER:CB	1:A:368:GLU:C	2.30	0.98
1:A:706:THR:OG1	1:A:710:GLN:NE2	2.06	0.89
1:A:899:ILE:HG22	1:A:907[B]:LEU:CD1	2.03	0.85
1:A:929:ARG:NH2	1:A:1001[B]:SER:OG	2.09	0.84
1:A:847:THR:HG22	3:A:2194:HOH:O	1.79	0.81
1:A:368:GLU:N	1:A:369:PRO:CD	2.46	0.78
1:A:962:ARG:HG2	1:A:962:ARG:HH11	1.51	0.75
1:A:367:SER:HB3	1:A:369:PRO:CA	2.16	0.75
1:A:367:SER:HA	1:A:368:GLU:CB	2.18	0.74
1:A:549:LEU:HG	1:A:564:MET:CE	2.17	0.74
1:A:902:ARG:HD2	3:A:2182:HOH:O	1.88	0.74
1:A:914:HIS:HB3	1:A:918:ASN:O	1.88	0.73
1:A:367:SER:HA	1:A:368:GLU:HB3	1.71	0.72
1:A:895:HIS:H	1:A:898:ASN:HD21	1.37	0.71
1:A:902:ARG:CD	3:A:2182:HOH:O	2.39	0.71
1:A:366:CYS:O	1:A:367:SER:CB	2.38	0.71
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.25	0.69
1:A:367:SER:C	1:A:369:PRO:HD3	2.13	0.68
1:A:610:GLN:OE1	1:A:795:GLN:NE2	2.26	0.68
1:A:899:ILE:HG23	1:A:907[B]:LEU:HD11	1.67	0.67
1:A:747:GLU:OE1	3:A:2127:HOH:O	2.12	0.67
1:A:110:LYS:NZ	1:A:144:ARG:HH12	1.94	0.65
1:A:900:MET:O	1:A:907[B]:LEU:HD12	1.97	0.65
1:A:929:ARG:HH22	1:A:1001[A]:SER:HB3	1.62	0.65
1:A:991:CYS:HB2	3:A:2238:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:THR:CG2	1:A:564:MET:HE2	2.27	0.64
1:A:553:THR:HG21	1:A:564:MET:HE2	1.79	0.64
1:A:786:GLN:OE1	3:A:2145:HOH:O	2.14	0.64
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.79	0.63
1:A:859:LEU:HD21	1:A:905:GLY:HA2	1.80	0.63
1:A:549:LEU:HG	1:A:564:MET:HE3	1.81	0.63
1:A:368:GLU:N	1:A:369:PRO:HD3	2.15	0.62
1:A:549:LEU:HG	1:A:564:MET:HE1	1.81	0.61
1:A:367:SER:HB3	1:A:369:PRO:CD	2.32	0.59
1:A:386:ARG:HG3	1:A:387:MET:CE	2.31	0.59
1:A:146:PHE:CE1	1:A:631:LYS:HD2	2.37	0.59
1:A:747:GLU:HG2	3:A:2128:HOH:O	2.01	0.59
1:A:679:MET:O	1:A:683:MET:HG3	2.03	0.59
1:A:366:CYS:O	1:A:367:SER:HB2	2.04	0.57
1:A:641:ARG:NH2	3:A:2082:HOH:O	2.39	0.56
1:A:367:SER:CB	1:A:368:GLU:O	2.54	0.56
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.88	0.55
1:A:895:HIS:H	1:A:898:ASN:ND2	2.03	0.55
1:A:617:GLN:HE22	1:A:620:LYS:NZ	2.05	0.55
1:A:435:GLY:HA2	1:A:475:LEU:O	2.08	0.54
1:A:329:GLU:HB2	1:A:369:PRO:O	2.08	0.53
1:A:902:ARG:HD3	3:A:2182:HOH:O	2.07	0.53
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.91	0.53
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.74	0.52
1:A:146:PHE:CZ	1:A:631:LYS:HD2	2.45	0.52
1:A:110:LYS:HZ1	1:A:144:ARG:HH12	1.58	0.51
1:A:329:GLU:HG2	1:A:472:VAL:CG2	2.41	0.51
1:A:367:SER:CA	1:A:368:GLU:CB	2.87	0.51
1:A:154:ARG:HD2	1:A:165:TYR:CZ	2.46	0.51
1:A:192:VAL:HG13	1:A:272:PRO:HB2	1.94	0.50
1:A:380:SER:HB3	1:A:383:ASP:OD1	2.11	0.50
1:A:154:ARG:HD2	1:A:165:TYR:CE2	2.47	0.50
1:A:170:GLN:HG2	3:A:2019:HOH:O	2.11	0.50
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.94	0.49
1:A:836[A]:ASN:HD22	2:A:1500:039:HAR	1.78	0.48
1:A:366:CYS:O	1:A:367:SER:OG	2.30	0.48
1:A:617:GLN:NE2	1:A:984:ALA:HA	2.29	0.48
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.95	0.48
1:A:962:ARG:HG2	1:A:962:ARG:NH1	2.26	0.47
1:A:895:HIS:ND1	1:A:897:ASP:OD1	2.47	0.47
1:A:386:ARG:HG3	1:A:387:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:THR:HG22	1:A:680:LYS:HE2	1.96	0.47
1:A:836[A]:ASN:ND2	2:A:1500:039:HAR	2.30	0.47
1:A:915:PHE:C	1:A:915:PHE:CD2	2.88	0.47
1:A:698:PHE:HZ	1:A:714:MET:HG2	1.80	0.47
1:A:617:GLN:HE22	1:A:620:LYS:HZ1	1.62	0.46
1:A:387:MET:HE2	1:A:590:CYS:SG	2.56	0.46
1:A:842:SER:O	1:A:844:MET:HG2	2.16	0.45
1:A:553:THR:CG2	1:A:564:MET:CE	2.93	0.45
1:A:367:SER:OG	1:A:368:GLU:O	2.30	0.45
1:A:620:LYS:HE2	1:A:660:VAL:HG11	1.99	0.45
1:A:278:HIS:HE1	3:A:2022:HOH:O	2.00	0.45
1:A:713:GLU:O	1:A:717:MET:HG3	2.16	0.44
1:A:698:PHE:HZ	1:A:714:MET:CG	2.29	0.44
1:A:832:ASP:OD2	1:A:836[B]:ASN:ND2	2.48	0.44
1:A:334:ASN:ND2	1:A:335:ALA:H	2.16	0.44
1:A:218:ALA:HB3	3:A:2021:HOH:O	2.17	0.43
1:A:736:ASP:CG	1:A:738:SER:HG	2.22	0.43
1:A:367:SER:CB	1:A:369:PRO:CA	2.91	0.43
1:A:553:THR:HG22	1:A:564:MET:HE2	2.00	0.43
1:A:169:LEU:HD22	1:A:259:PHE:HE1	1.84	0.43
1:A:289:GLN:HG2	1:A:677:HIS:CD2	2.53	0.43
1:A:191:LEU:O	1:A:272:PRO:HD2	2.18	0.43
1:A:895:HIS:CE1	1:A:898:ASN:OD1	2.72	0.43
1:A:735:LEU:HD11	1:A:824:LEU:HB3	2.00	0.42
1:A:328:ILE:HD11	1:A:474:TYR:HB2	2.01	0.42
1:A:245:GLY:HA3	1:A:768:ALA:HB2	2.02	0.42
1:A:368:GLU:N	1:A:369:PRO:HD2	2.28	0.42
1:A:1023:LEU:O	1:A:1026:SER:HB3	2.20	0.42
1:A:213:PRO:HD3	1:A:254:TYR:O	2.20	0.42
1:A:110:LYS:HZ3	1:A:144:ARG:HH12	1.63	0.41
1:A:135:GLU:HG2	1:A:625:LEU:HD12	2.02	0.41
1:A:929:ARG:HH22	1:A:1001[A]:SER:CB	2.25	0.41
1:A:213:PRO:O	1:A:217:MET:HG3	2.20	0.41
1:A:784:LEU:HD12	1:A:823:GLY:HA3	2.02	0.41
1:A:846:ALA:HA	1:A:857:ASN:HB3	2.03	0.40
1:A:758:PRO:HB3	1:A:779:LYS:HG2	2.03	0.40
1:A:332:LYS:HE3	1:A:333:VAL:N	2.36	0.40
1:A:208:SER:OG	1:A:210:LYS:HG2	2.21	0.40
1:A:367:SER:CB	1:A:369:PRO:HA	2.51	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)
1:A:714:MET:CE	1:A:714:MET:CE[2_555]	1.79	0.41

## 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	805/940 (86%)	788 (98%)	15 (2%)	2 (0%)	52 42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	SER
1	A	742	GLU

### 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	733/827 (89%)	691 (94%)	42 (6%)	25 13

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	188	ARG
1	A	190	LEU
1	A	291	ASN

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Mol	Chain	Res	Type
1	A	316	LEU
1	A	317	TRP
1	A	331	ARG
1	A	332	LYS
1	A	340	LYS
1	A	352	GLU
1	A	368	GLU
1	A	394	LEU
1	A	397	VAL
1	A	423	LEU
1	A	445	VAL
1	A	453	LEU
1	A	511	LEU
1	A	514	ILE
1	A	517	ARG
1	A	523	LEU
1	A	525	GLU
1	A	530	LEU
1	A	553	THR
1	A	560	ASP
1	A	565	LEU
1	A	631	LYS
1	A	634	LEU
1	A	705	LYS
1	A	706	THR
1	A	714	MET
1	A	757	LYS
1	A	795	GLN
1	A	855	LEU
1	A	895	HIS
1	A	898	ASN
1	A	915	PHE
1	A	937	ASP
1	A	962	ARG
1	A	986	LEU
1	A	990	SER
1	A	1004	LEU
1	A	1009	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	170	GLN
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	334	ASN
1	A	351	ASN
1	A	617	GLN
1	A	710	GLN
1	A	780	ASN
1	A	898	ASN

### 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](#)

1 ligand 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	$\# Z  > 2$
2	039	A	1500	-	32,35,35	1.58	4 (12%)	31,50,50	3.07	9 (29%)

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	039	A	1500	-	-	0/9/11/11	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	039	C6-C5	-5.50	1.39	1.43
2	A	1500	039	CAH-CAP	-2.94	1.36	1.43
2	A	1500	039	CAH-NAG	-2.47	1.42	1.45
2	A	1500	039	CAS-CAO	2.53	1.53	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	039	N3-C2-N1	-10.56	120.81	128.89
2	A	1500	039	CAU-OAT-CAP	-9.06	103.80	117.54
2	A	1500	039	CAI-CAH-NAG	-2.61	115.13	118.50
2	A	1500	039	CAF-CAE-CAD	-2.01	123.51	126.72
2	A	1500	039	CAO-CAS-S6	2.05	112.50	109.25
2	A	1500	039	C2-N1-C6	2.35	121.41	116.47
2	A	1500	039	CAS-CAO-NAN	3.26	121.97	116.36
2	A	1500	039	S6-C6-N1	4.58	126.69	117.59
2	A	1500	039	CAP-CAH-NAG	5.23	123.24	118.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	039	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	822/940 (87%)	0.95	140 (17%) 2 2	5, 17, 32, 49	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	ASN	8.2
1	A	228	PHE	8.2
1	A	317	TRP	7.9
1	A	341	LEU	7.6
1	A	919	PHE	7.4
1	A	366	CYS	7.3
1	A	330	GLY	6.5
1	A	484	TYR	6.2
1	A	342	VAL	6.0
1	A	377	PHE	5.8
1	A	363	VAL	5.8
1	A	319	LEU	5.6
1	A	445	VAL	5.1
1	A	512	ARG	4.9
1	A	395	TYR	4.7
1	A	522	GLU	4.5
1	A	398	VAL	4.5
1	A	843	ASN	4.5
1	A	370	VAL	4.5
1	A	361	SER	4.4
1	A	514	ILE	4.4
1	A	1027	TRP	4.4
1	A	340	LYS	4.4
1	A	542	PHE	4.4
1	A	397	VAL	4.3
1	A	396	ALA	4.3
1	A	511	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	472	VAL	4.2
1	A	616	VAL	4.2
1	A	367	SER	4.0
1	A	205	PHE	3.9
1	A	846	ALA	3.9
1	A	647	LEU	3.9
1	A	529	ASP	3.8
1	A	493	GLU	3.8
1	A	612	LEU	3.8
1	A	332	LYS	3.7
1	A	339	MET	3.7
1	A	394	LEU	3.7
1	A	187	ASN	3.6
1	A	651	LEU	3.6
1	A	847	THR	3.6
1	A	191	LEU	3.5
1	A	466	GLU	3.5
1	A	534	MET	3.5
1	A	364	ASN	3.5
1	A	227	VAL	3.4
1	A	619	LEU	3.4
1	A	474	TYR	3.4
1	A	188	ARG	3.4
1	A	365	VAL	3.4
1	A	189	ALA	3.3
1	A	373	GLN	3.3
1	A	646	PHE	3.3
1	A	936	TYR	3.3
1	A	333	VAL	3.3
1	A	492	LEU	3.2
1	A	416	CYS	3.2
1	A	613	LEU	3.2
1	A	488	LEU	3.2
1	A	609	PHE	3.1
1	A	444	SER	3.1
1	A	913	GLY	3.1
1	A	489	GLU	3.1
1	A	526	HIS	3.0
1	A	491	ILE	3.0
1	A	541	HIS	2.9
1	A	374	ARG	2.9
1	A	329	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	570	SER	2.9
1	A	372	LYS	2.9
1	A	530	LEU	2.9
1	A	362	GLU	2.8
1	A	643	ILE	2.8
1	A	478	VAL	2.8
1	A	368	GLU	2.7
1	A	210	LYS	2.7
1	A	323	PHE	2.7
1	A	375	LEU	2.7
1	A	418	ILE	2.7
1	A	634	LEU	2.7
1	A	322	PRO	2.7
1	A	200	GLU	2.7
1	A	538	VAL	2.7
1	A	615	LEU	2.7
1	A	845	ALA	2.6
1	A	230	GLN	2.6
1	A	515	LEU	2.6
1	A	735	LEU	2.6
1	A	109	VAL	2.6
1	A	618	VAL	2.6
1	A	524	TYR	2.5
1	A	633	LEU	2.5
1	A	525	GLU	2.5
1	A	190	LEU	2.5
1	A	980	LEU	2.5
1	A	206	GLN	2.4
1	A	318	SER	2.4
1	A	477	GLU	2.4
1	A	517	ARG	2.4
1	A	776	ILE	2.4
1	A	417	PRO	2.3
1	A	816	LEU	2.3
1	A	479	ALA	2.3
1	A	465	THR	2.3
1	A	475	LEU	2.3
1	A	1017	VAL	2.3
1	A	458	THR	2.3
1	A	566	TYR	2.3
1	A	848	ALA	2.3
1	A	649	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	718[A]	CYS	2.2
1	A	384	LEU	2.2
1	A	235	GLN	2.2
1	A	371	TRP	2.2
1	A	895	HIS	2.2
1	A	132	ARG	2.2
1	A	229	ARG	2.2
1	A	893	ASP	2.1
1	A	327	LEU	2.1
1	A	1005	GLY	2.1
1	A	226	THR	2.1
1	A	467	SER	2.1
1	A	667	ILE	2.1
1	A	459	VAL	2.1
1	A	383	ASP	2.1
1	A	648	PHE	2.1
1	A	222	ARG	2.1
1	A	1013	LYS	2.1
1	A	369	PRO	2.1
1	A	815	CYS	2.1
1	A	270	LEU	2.1
1	A	432	LEU	2.1
1	A	469	ALA	2.1
1	A	203	PHE	2.1
1	A	325	ILE	2.1
1	A	791	LEU	2.0
1	A	328	ILE	2.0
1	A	650	HIS	2.0
1	A	774	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

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( $\text{\AA}^2$ )	Q<0.9
2	039	A	1500	31/31	0.94	0.12	-0.35	20,25,35,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.