



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:33 PM GMT

PDB ID : 3ZVV  
Title : FRAGMENT BOUND TO PI3KINASE GAMMA  
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Deposited on : 2011-07-27  
Resolution : 2.50 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

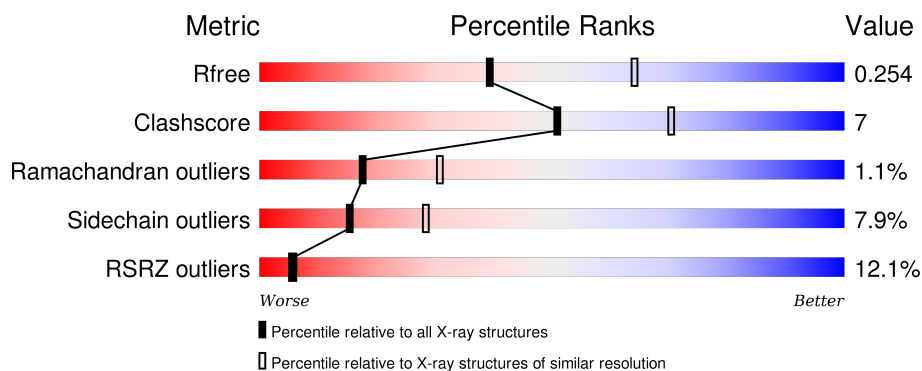
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	966	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7023 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.

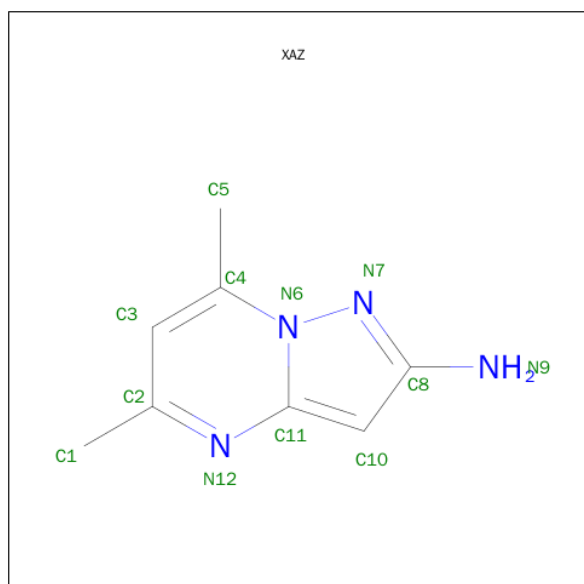
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	829	Total	C	N	O	S	0	0	0
			6724	4319	1150	1220	35			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	EXPRESSION TAG	UNP P48736
A	1103	HIS	-	EXPRESSION TAG	UNP P48736
A	1104	HIS	-	EXPRESSION TAG	UNP P48736
A	1105	HIS	-	EXPRESSION TAG	UNP P48736
A	1106	HIS	-	EXPRESSION TAG	UNP P48736
A	1107	HIS	-	EXPRESSION TAG	UNP P48736
A	1108	HIS	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is 5,7-DIMETHYLPYRAZOLO[1,5-A]PYRIMIDIN-2-AMINE (three-letter code: XAZ) (formula: C<sub>8</sub>H<sub>10</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			12	8	4		

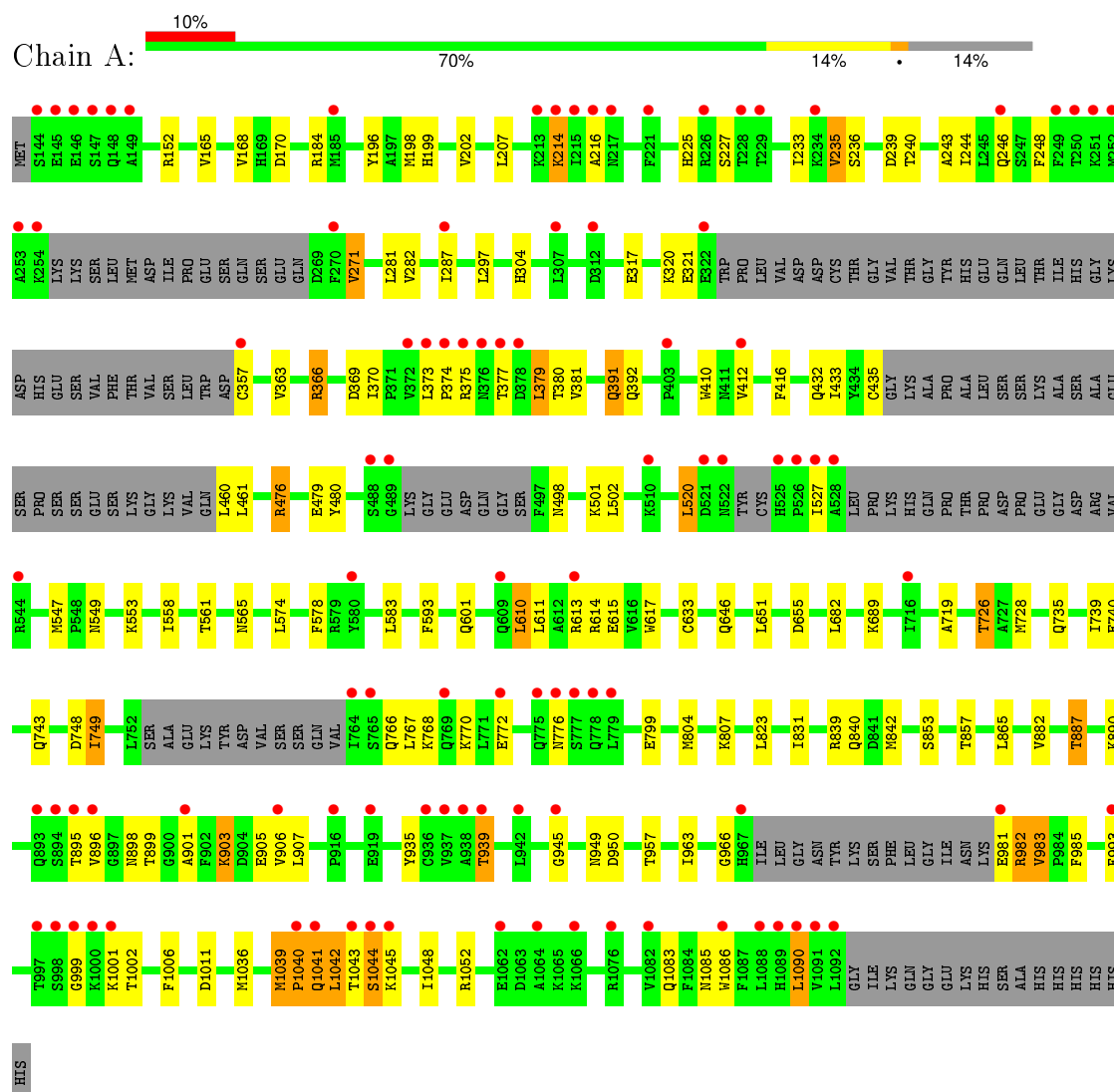
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	287	Total	O	0	0
			287	287		

### 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 errors 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-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.49 Å 68.03 Å 106.25 Å 90.00° 95.16° 90.00°	Depositor
Resolution (Å)	16.62 – 2.50 28.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (16.62-2.50) 99.0 (28.61-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.51 Å)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
R, $R_{free}$	0.192 , 0.242 0.202 , 0.254	Depositor DCC
$R_{free}$ test set	1751 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 62.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 35189 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7023	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAZ

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	0.50	0/6868	0.65	0/9288

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6724	0	6768	93	0
2	A	12	0	10	3	0
3	A	287	0	0	4	0
All	All	7023	0	6778	93	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 7.

All (93) 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:689:LYS:HG2	1:A:728:MET:HE2	1.30	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.49	0.94
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.14	0.93
1:A:689:LYS:HG2	1:A:728:MET:CE	2.00	0.91
1:A:839:ARG:HA	1:A:842:MET:HE2	1.50	0.90
1:A:689:LYS:CG	1:A:728:MET:HE2	2.01	0.90
1:A:235:VAL:HG21	1:A:244:ILE:HG12	1.56	0.87
1:A:935:TYR:O	1:A:939:THR:HB	1.77	0.84
1:A:804:MET:HE1	1:A:831:ILE:HG12	1.65	0.79
1:A:939:THR:HG23	1:A:945:GLY:CA	2.14	0.77
1:A:804:MET:CE	1:A:831:ILE:HG12	2.14	0.77
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.34	0.74
1:A:887:THR:HG22	1:A:890:LYS:H	1.53	0.73
1:A:199:HIS:HD2	3:A:2028:HOH:O	1.72	0.72
1:A:225:HIS:HE1	1:A:304:HIS:CD2	2.04	0.72
1:A:882:VAL:HG23	2:A:1500:XAZ:H51C	1.73	0.70
1:A:558:ILE:O	1:A:561:THR:HG22	1.92	0.69
1:A:271:VAL:CG2	1:A:282:VAL:HG11	2.22	0.68
1:A:214:LYS:HD3	1:A:297:LEU:O	1.97	0.65
1:A:391:GLN:NE2	1:A:633:CYS:HB2	2.12	0.65
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.82	0.62
1:A:1040:PRO:HB3	3:A:2112:HOH:O	1.98	0.61
1:A:689:LYS:CD	1:A:728:MET:HE2	2.30	0.61
1:A:939:THR:CG2	1:A:945:GLY:HA2	2.25	0.60
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.67	0.60
1:A:1043:THR:C	1:A:1045:LYS:H	2.05	0.59
1:A:271:VAL:CG2	1:A:282:VAL:CG1	2.81	0.59
1:A:240:THR:HG23	1:A:243:ALA:H	1.67	0.59
1:A:196:TYR:OH	1:A:728:MET:HE3	2.03	0.58
1:A:963:ILE:HB	2:A:1500:XAZ:H13C	1.86	0.57
1:A:981:GLU:HA	1:A:982:ARG:CZ	2.36	0.56
1:A:804:MET:HE3	1:A:831:ILE:HG12	1.89	0.55
1:A:381:VAL:CG2	1:A:433:ILE:HG23	2.38	0.54
1:A:768:LYS:O	1:A:772:GLU:HG2	2.07	0.54
1:A:460:LEU:HD21	1:A:501:LYS:HZ3	1.73	0.54
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.42	0.53
1:A:246:GLN:HE21	1:A:246:GLN:HA	1.74	0.53
1:A:235:VAL:CG2	1:A:244:ILE:HG12	2.35	0.52
1:A:905:GLU:HG3	1:A:993:PHE:CE2	2.45	0.52
1:A:903:LYS:HB3	1:A:906:VAL:HG23	1.91	0.52
1:A:271:VAL:HG22	1:A:282:VAL:CG1	2.38	0.52
1:A:882:VAL:HG23	2:A:1500:XAZ:C5	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:SER:HA	1:A:1048:ILE:HD12	1.93	0.51
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.92	0.51
1:A:168:VAL:HG13	1:A:170:ASP:O	2.10	0.51
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.07	0.51
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.07	0.50
1:A:549:ASN:O	1:A:553:LYS:HG3	2.11	0.49
1:A:728:MET:HE1	3:A:2024:HOH:O	2.13	0.49
1:A:196:TYR:OH	1:A:728:MET:CE	2.61	0.48
1:A:1042:LEU:CD1	1:A:1042:LEU:H	2.26	0.48
1:A:317:GLU:O	1:A:726:THR:CG2	2.62	0.48
1:A:748:ASP:HB3	1:A:770:LYS:NZ	2.29	0.48
1:A:749:ILE:CD1	1:A:770:LYS:HD2	2.44	0.47
1:A:1002:THR:HG23	1:A:1006:PHE:HD2	1.79	0.47
1:A:432:GLN:OE1	1:A:501:LYS:NZ	2.39	0.47
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.96	0.47
1:A:476:ARG:HB3	1:A:520:LEU:HD23	1.96	0.47
1:A:239:ASP:O	1:A:287:ILE:HG13	2.13	0.47
1:A:184:ARG:HD3	1:A:719:ALA:O	2.14	0.47
1:A:547:MET:HG2	1:A:578:PHE:CD1	2.50	0.47
1:A:1042:LEU:HD13	1:A:1042:LEU:H	1.80	0.46
1:A:317:GLU:O	1:A:726:THR:HG23	2.16	0.46
1:A:735:GLN:O	1:A:739:ILE:HG23	2.16	0.46
1:A:1036:MET:HA	1:A:1042:LEU:HD11	1.98	0.45
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.98	0.45
1:A:366:ARG:NH1	1:A:479:GLU:OE1	2.49	0.45
1:A:804:MET:HE3	1:A:831:ILE:HG23	1.97	0.45
1:A:391:GLN:HE22	1:A:502:LEU:HD11	1.82	0.45
1:A:887:THR:HG21	1:A:950:ASP:OD1	2.18	0.44
1:A:379:LEU:HD23	1:A:380:THR:HG22	1.99	0.44
1:A:749:ILE:HD12	1:A:770:LYS:HD2	2.00	0.44
1:A:1040:PRO:O	1:A:1042:LEU:HD12	2.18	0.43
1:A:363:VAL:HG23	1:A:520:LEU:CD1	2.48	0.43
1:A:233:ILE:HD12	1:A:248:PHE:HD1	1.83	0.43
1:A:476:ARG:HG3	1:A:480:TYR:OH	2.19	0.43
1:A:593:PHE:HZ	1:A:611:LEU:HD21	1.83	0.43
1:A:739:ILE:HG13	1:A:740:GLU:N	2.33	0.43
1:A:840:GLN:HG2	1:A:1039:MET:HE2	1.99	0.43
1:A:236:SER:O	1:A:287:ILE:HD11	2.19	0.42
1:A:898:ASN:HB2	1:A:901:ALA:HB3	2.01	0.42
1:A:271:VAL:HG21	1:A:282:VAL:HG11	2.00	0.42
1:A:391:GLN:HE22	1:A:633:CYS:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:PHE:HA	3:A:2135:HOH:O	2.20	0.42
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.85	0.41
1:A:1043:THR:O	1:A:1045:LYS:N	2.54	0.41
1:A:903:LYS:NZ	1:A:905:GLU:HB3	2.36	0.41
1:A:983:VAL:HG13	1:A:985:PHE:O	2.20	0.41
1:A:198:MET:SD	1:A:271:VAL:HG21	2.61	0.40
1:A:1086:TRP:CD1	1:A:1090:LEU:HG	2.56	0.40
1:A:853:SER:O	1:A:857:THR:HG23	2.21	0.40
1:A:1042:LEU:CD1	1:A:1042:LEU:N	2.85	0.40
1:A:1041:GLN:HA	1:A:1041:GLN:HE21	1.87	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	811/966 (84%)	777 (96%)	25 (3%)	9 (1%)	17	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ALA
1	A	374	PRO
1	A	899	THR
1	A	1040	PRO
1	A	896	VAL
1	A	1044	SER
1	A	999	GLY
1	A	227	SER
1	A	966	GLY

### 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	744/864 (86%)	685 (92%)	59 (8%)	15	28

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	ARG
1	A	165	VAL
1	A	202	VAL
1	A	207	LEU
1	A	214	LYS
1	A	235	VAL
1	A	271	VAL
1	A	281	LEU
1	A	320	LYS
1	A	321	GLU
1	A	357	CYS
1	A	366	ARG
1	A	369	ASP
1	A	370	ILE
1	A	373	LEU
1	A	375	ARG
1	A	377	THR
1	A	379	LEU
1	A	391	GLN
1	A	392	GLN
1	A	435	CYS
1	A	461	LEU
1	A	476	ARG
1	A	498	ASN
1	A	520	LEU
1	A	527	ILE
1	A	574	LEU
1	A	601	GLN
1	A	610	LEU
1	A	613	ARG

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Mol	Chain	Res	Type
1	A	615	GLU
1	A	646	GLN
1	A	682	LEU
1	A	726	THR
1	A	743	GLN
1	A	749	ILE
1	A	766	GLN
1	A	767	LEU
1	A	776	ASN
1	A	799	GLU
1	A	807	LYS
1	A	823	LEU
1	A	865	LEU
1	A	887	THR
1	A	895	THR
1	A	903	LYS
1	A	907	LEU
1	A	939	THR
1	A	957	THR
1	A	982	ARG
1	A	983	VAL
1	A	1001	LYS
1	A	1011	ASP
1	A	1039	MET
1	A	1041	GLN
1	A	1042	LEU
1	A	1052	ARG
1	A	1085	ASN
1	A	1090	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	HIS
1	A	246	GLN
1	A	304	HIS
1	A	389	HIS
1	A	391	GLN
1	A	392	GLN
1	A	565	ASN
1	A	601	GLN
1	A	646	GLN

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Mol	Chain	Res	Type
1	A	743	GLN
1	A	834	HIS
1	A	959	ASN
1	A	1023	HIS
1	A	1041	GLN
1	A	1083	GLN
1	A	1085	ASN

### 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 ⓘ

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	XAZ	A	1500	-	8,13,13	4.69	6 (75%)	8,19,19	4.30	5 (62%)

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	XAZ	A	1500	-	-	0/0/0/0	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	XAZ	C5-C4	-7.59	1.41	1.50
2	A	1500	XAZ	C8-N7	-4.01	1.28	1.34
2	A	1500	XAZ	C8-N9	2.36	1.42	1.35
2	A	1500	XAZ	C1-C2	2.62	1.56	1.50
2	A	1500	XAZ	C2-N12	3.84	1.41	1.33
2	A	1500	XAZ	C11-N12	8.50	1.44	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	XAZ	C3-C2-N12	-8.54	115.34	122.69
2	A	1500	XAZ	C5-C4-C3	-2.73	116.55	122.37
2	A	1500	XAZ	C1-C2-C3	-2.59	118.27	121.75
2	A	1500	XAZ	C2-N12-C11	5.07	124.07	117.71
2	A	1500	XAZ	C1-C2-N12	5.24	126.39	117.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	XAZ	3	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	829/966 (85%)	0.64	100 (12%) 6 5	34, 76, 138, 196	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1092	LEU	10.5
1	A	1044	SER	10.3
1	A	1091	VAL	7.9
1	A	377	THR	7.5
1	A	895	THR	7.1
1	A	374	PRO	6.8
1	A	253	ALA	6.4
1	A	254	LYS	6.2
1	A	1086	TRP	6.2
1	A	376	ASN	6.1
1	A	216	ALA	6.0
1	A	776	ASN	5.7
1	A	1088	LEU	5.7
1	A	1089	HIS	5.6
1	A	378	ASP	5.1
1	A	528	ALA	5.1
1	A	322	GLU	5.1
1	A	217	ASN	5.1
1	A	146	GLU	4.8
1	A	526	PRO	4.7
1	A	148	GLN	4.7
1	A	778	GLN	4.7
1	A	373	LEU	4.5
1	A	375	ARG	4.3
1	A	998	SER	4.3
1	A	147	SER	4.2
1	A	228	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	249	PHE	4.2
1	A	967	HIS	4.1
1	A	896	VAL	4.0
1	A	544	ARG	4.0
1	A	270	PHE	4.0
1	A	1043	THR	3.8
1	A	250	THR	3.8
1	A	251	LYS	3.7
1	A	919	GLU	3.7
1	A	1064	ALA	3.6
1	A	246	GLN	3.6
1	A	777	SER	3.6
1	A	489	GLY	3.5
1	A	145	GLU	3.5
1	A	1000	LYS	3.5
1	A	525	HIS	3.5
1	A	226	ARG	3.4
1	A	1045	LYS	3.4
1	A	997	THR	3.4
1	A	993	PHE	3.3
1	A	916	PRO	3.3
1	A	764	ILE	3.3
1	A	252	MET	3.2
1	A	149	ALA	3.1
1	A	981	GLU	3.0
1	A	938	ALA	3.0
1	A	894	SER	3.0
1	A	945	GLY	3.0
1	A	906	VAL	2.9
1	A	772	GLU	2.9
1	A	1062	GLU	2.9
1	A	939	THR	2.9
1	A	937	VAL	2.9
1	A	403	PRO	2.8
1	A	312	ASP	2.7
1	A	521	ASP	2.7
1	A	1001	LYS	2.7
1	A	1082	VAL	2.7
1	A	779	LEU	2.6
1	A	769	GLN	2.6
1	A	213	LYS	2.6
1	A	234	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1041	GLN	2.6
1	A	901	ALA	2.5
1	A	999	GLY	2.5
1	A	1040	PRO	2.5
1	A	357	CYS	2.5
1	A	488	SER	2.4
1	A	613	ARG	2.4
1	A	307	LEU	2.4
1	A	144	SER	2.4
1	A	221	PHE	2.4
1	A	1090	LEU	2.4
1	A	510	LYS	2.3
1	A	412	VAL	2.3
1	A	893	GLN	2.3
1	A	229	THR	2.3
1	A	215	ILE	2.3
1	A	580	TYR	2.3
1	A	775	GLN	2.3
1	A	287	ILE	2.2
1	A	527	ILE	2.2
1	A	609	GLN	2.2
1	A	372	VAL	2.2
1	A	1066	LYS	2.2
1	A	1076	ARG	2.2
1	A	522	ASN	2.2
1	A	942	LEU	2.1
1	A	936	CYS	2.1
1	A	765	SER	2.1
1	A	185	MET	2.1
1	A	716	ILE	2.0
1	A	214	LYS	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	XAZ	A	1500	12/12	0.98	0.14	0.04	51,59,60,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.