



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:09 AM GMT

PDB ID : 3L16  
Title : Discovery of (thienopyrimidin-2-yl)aminopyrimidines as Potent, Selective, and Orally Available Pan-PI3-Kinase and Dual Pan-PI3-Kinase/mTOR Inhibitors for the Treatment of Cancer  
Authors : Murray, J.M.; Wiesmann, C.  
Deposited on : 2009-12-10  
Resolution : 2.90 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

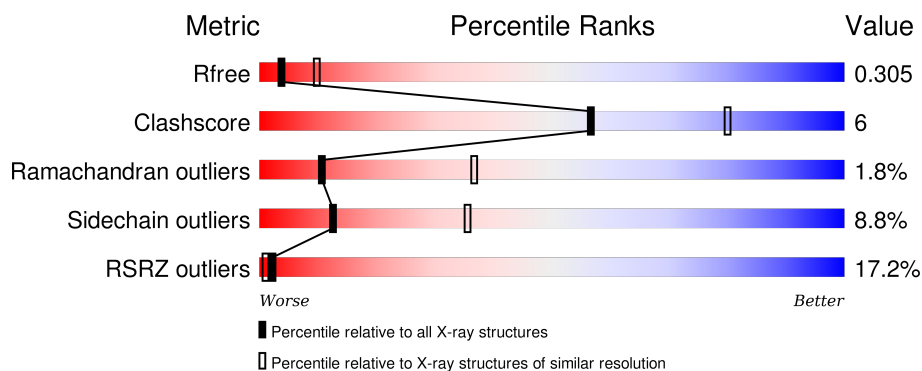
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	966	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6845 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.

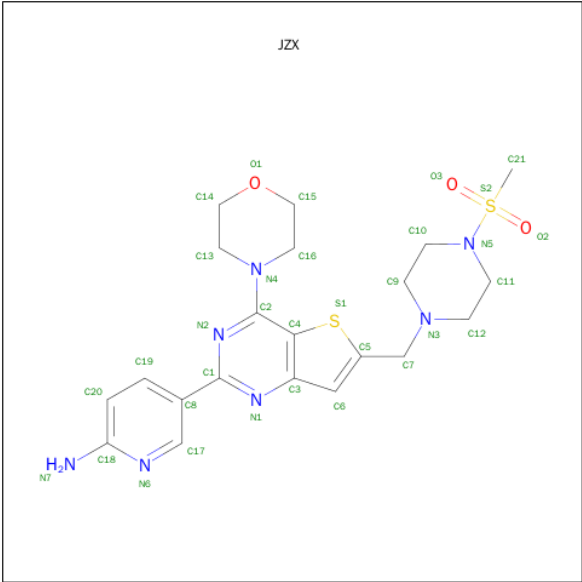
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6812	4371	1164	1242	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-(6-([4-(METHYLSULFONYL)PIPERAZIN-1-YL]METHYL)-4-MORPHOLIN-4-YLTHIENO[3,2-D]PYRIMIDIN-2-YL)PYRIDIN-2-AMINE (three-letter code: JZX) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			33	21	7	3	2		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.63Å 67.39Å 106.67Å 90.00° 96.11° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-2.90) 98.1 (19.75-2.90)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.99 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.238 , 0.295 0.269 , 0.305	Depositor DCC
$R_{free}$ test set	1125 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.6	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 94.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 22093 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6845	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: JZX

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	0.48	0/6958	0.63	1/9412 (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
1	A	0	2

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	641	ARG	NE-CZ-NH1	-5.91	117.35	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	756	LYS	Peptide
1	A	807	LYS	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	6812	0	6843	82	0
2	A	33	0	27	2	0
All	All	6845	0	6870	83	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 6.

All (83) 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:548:PRO:O	1:A:550:GLN:N	2.20	0.73
1:A:395:CYS:SG	1:A:417:SER:OG	2.46	0.73
1:A:867:TYR:CE2	1:A:963:ILE:HG22	2.28	0.68
1:A:583:LEU:HD13	1:A:610:LEU:HD22	1.77	0.66
1:A:425:LYS:NZ	1:A:473:PHE:CZ	2.56	0.65
1:A:635:PHE:O	1:A:641:ARG:HD2	1.99	0.63
2:A:1:JZX:S1	2:A:1:JZX:H16A	2.38	0.63
1:A:1056:THR:HG23	1:A:1056:THR:O	1.99	0.63
1:A:428:LEU:HD23	1:A:467:LEU:HD23	1.81	0.62
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.48	0.61
1:A:706:SER:O	1:A:710:GLN:HB3	2.02	0.59
1:A:1030:LEU:O	1:A:1031:PHE:C	2.39	0.59
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.02	0.58
1:A:743:GLN:HE21	1:A:876:ILE:HG12	1.68	0.58
1:A:806:SER:OG	1:A:807:LYS:N	2.37	0.58
1:A:525:HIS:HB3	1:A:526:PRO:HD3	1.86	0.57
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.86	0.57
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.87	0.56
1:A:576:TRP:O	1:A:579:ARG:HD3	2.04	0.55
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.88	0.55
1:A:897:GLY:O	1:A:899:THR:N	2.40	0.55
1:A:847:ILE:O	1:A:850:ILE:N	2.41	0.53
1:A:802:LYS:HE2	2:A:1:JZX:O2	2.08	0.52
1:A:734:GLN:OE1	1:A:780:PRO:HB3	2.09	0.52
1:A:1056:THR:CG2	1:A:1056:THR:O	2.58	0.51
1:A:233:ILE:HG22	1:A:235:VAL:HG23	1.94	0.50
1:A:703:ILE:HD11	1:A:714:ALA:HA	1.94	0.49
1:A:373:LEU:N	1:A:374:PRO:CD	2.75	0.49
1:A:564:LEU:HD11	1:A:1048:ILE:CG2	2.42	0.49
1:A:363:VAL:HG23	1:A:520:LEU:CD1	2.43	0.49
1:A:628:MET:O	1:A:631:LEU:N	2.41	0.49
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:PHE:O	1:A:736:VAL:HG23	2.14	0.48
1:A:1086:TRP:O	1:A:1087:PHE:HB2	2.14	0.47
1:A:947:ARG:NH2	1:A:964:ASP:O	2.47	0.47
1:A:209:GLU:HB2	1:A:859:SER:HB3	1.95	0.47
1:A:1086:TRP:CH2	1:A:1090:LEU:HD11	2.50	0.47
1:A:799:GLU:CD	1:A:799:GLU:H	2.17	0.47
1:A:498:ASN:OD1	1:A:498:ASN:C	2.53	0.47
1:A:239:ASP:HB3	1:A:244:ILE:HG23	1.97	0.47
1:A:641:ARG:NE	1:A:670:GLU:OE1	2.41	0.46
1:A:363:VAL:HG13	1:A:363:VAL:O	2.16	0.46
1:A:988:THR:HG21	1:A:1083:GLN:HG3	1.98	0.46
1:A:887:THR:HG22	1:A:889:ALA:N	2.31	0.45
1:A:893:GLN:O	1:A:894:SER:C	2.54	0.45
1:A:804:MET:HE1	1:A:831:ILE:HG23	1.98	0.45
1:A:425:LYS:NZ	1:A:473:PHE:CE2	2.80	0.45
1:A:283:GLY:O	1:A:285:THR:N	2.49	0.45
1:A:947:ARG:NH2	1:A:963:ILE:O	2.49	0.45
1:A:1086:TRP:O	1:A:1087:PHE:CB	2.64	0.45
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.99	0.44
1:A:608:TYR:OH	1:A:637:ASP:OD2	2.29	0.44
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.52	0.44
1:A:690:ARG:O	1:A:694:PHE:HD1	2.01	0.44
1:A:284:GLU:HA	1:A:284:GLU:OE1	2.18	0.43
1:A:766:GLN:HB3	1:A:766:GLN:HE21	1.61	0.43
1:A:785:VAL:HG23	1:A:791:LEU:O	2.19	0.43
1:A:646:GLN:HB3	1:A:646:GLN:HE21	1.69	0.43
1:A:834:HIS:HB2	1:A:876:ILE:HD12	2.01	0.43
1:A:1064:ALA:O	1:A:1065:LYS:C	2.57	0.43
1:A:1030:LEU:O	1:A:1032:SER:N	2.52	0.43
1:A:891:ILE:O	1:A:906:VAL:HG11	2.19	0.43
1:A:470:ASP:C	1:A:470:ASP:OD1	2.57	0.43
1:A:829:GLY:HA3	1:A:881:ILE:HB	2.01	0.42
1:A:226:ARG:O	1:A:228:THR:N	2.52	0.42
1:A:466:LEU:HD11	1:A:476:ARG:HD3	2.00	0.42
1:A:717:LEU:HD22	1:A:721:LEU:HG	2.01	0.42
1:A:429:LEU:HB2	1:A:468:LEU:HD21	2.00	0.42
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.54	0.42
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	2.01	0.42
1:A:948:HIS:CD2	1:A:950:ASP:HB2	2.55	0.42
1:A:144:SER:HB3	1:A:147:SER:HB2	2.02	0.42
1:A:865:LEU:HA	1:A:865:LEU:HD12	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PRO:HA	1:A:287:ILE:HD11	2.01	0.41
1:A:983:VAL:HG22	1:A:984:PRO:HD2	2.02	0.41
1:A:462:TYR:HA	1:A:485:TRP:O	2.20	0.41
1:A:639:ASN:O	1:A:640:VAL:C	2.56	0.41
1:A:887:THR:CG2	1:A:889:ALA:HB3	2.51	0.41
1:A:885:ALA:HA	1:A:955:THR:HA	2.03	0.41
1:A:847:ILE:O	1:A:848:LEU:C	2.59	0.40
1:A:160:TYR:OH	1:A:711:GLN:HG2	2.20	0.40
1:A:648:LEU:O	1:A:650:SER:N	2.55	0.40
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.57	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	825/966 (85%)	721 (87%)	89 (11%)	15 (2%)	11 37

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	549	ASN
1	A	894	SER
1	A	898	ASN
1	A	1040	PRO
1	A	1087	PHE
1	A	284	GLU
1	A	471	HIS
1	A	899	THR
1	A	964	ASP
1	A	227	SER
1	A	374	PRO

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Mol	Chain	Res	Type
1	A	848	LEU
1	A	526	PRO
1	A	896	VAL
1	A	999	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	754/864 (87%)	688 (91%)	66 (9%)	12	35

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	146	GLU
1	A	152	ARG
1	A	202	VAL
1	A	213	LYS
1	A	219	CYS
1	A	226	ARG
1	A	252	MET
1	A	267	GLU
1	A	278	ASP
1	A	281	LEU
1	A	282	VAL
1	A	306	VAL
1	A	309	THR
1	A	369	ASP
1	A	375	ARG
1	A	379	LEU
1	A	381	VAL
1	A	391	GLN
1	A	395	CYS
1	A	421	LYS
1	A	520	LEU

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Mol	Chain	Res	Type
1	A	549	ASN
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU
1	A	583	LEU
1	A	610	LEU
1	A	626	LEU
1	A	646	GLN
1	A	647	LYS
1	A	662	GLN
1	A	682	LEU
1	A	717	LEU
1	A	731	ASP
1	A	764	ILE
1	A	766	GLN
1	A	807	LYS
1	A	808	LYS
1	A	823	LEU
1	A	833	LYS
1	A	838	LEU
1	A	841	ASP
1	A	845	LEU
1	A	865	LEU
1	A	870	ILE
1	A	871	SER
1	A	883	LYS
1	A	894	SER
1	A	898	ASN
1	A	899	THR
1	A	903	LYS
1	A	907	LEU
1	A	918	GLU
1	A	988	THR
1	A	1026	LEU
1	A	1029	ILE
1	A	1042	LEU
1	A	1043	THR
1	A	1048	ILE
1	A	1049	GLU
1	A	1052	ARG
1	A	1056	THR
1	A	1078	LYS

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Mol	Chain	Res	Type
1	A	1084	PHE
1	A	1090	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	291	GLN
1	A	391	GLN
1	A	646	GLN
1	A	705	GLN
1	A	743	GLN
1	A	766	GLN
1	A	769	GLN
1	A	775	GLN
1	A	825	ASN
1	A	834	HIS
1	A	898	ASN
1	A	1007	GLN
1	A	1083	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 [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	JZX	A	1	-	35,37,37	1.47	4 (11%)	43,54,54	2.66	15 (34%)

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	JZX	A	1	-	-	0/17/36/36	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	JZX	C21-S2	-4.45	1.67	1.75
2	A	1	JZX	C6-C5	-3.91	1.27	1.37
2	A	1	JZX	C5-S1	-3.26	1.68	1.74
2	A	1	JZX	C6-C3	-3.11	1.29	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	JZX	N1-C1-N2	-8.53	120.70	126.20
2	A	1	JZX	O3-S2-O2	-6.16	110.09	118.66
2	A	1	JZX	C11-N5-S2	-4.95	110.81	115.99
2	A	1	JZX	C10-N5-S2	-3.79	112.03	115.99
2	A	1	JZX	C15-C16-N4	-3.45	103.93	110.02
2	A	1	JZX	C4-C2-N2	-2.68	116.58	122.40
2	A	1	JZX	C8-C17-N6	-2.63	120.09	124.34
2	A	1	JZX	C12-C11-N5	-2.27	107.18	109.02
2	A	1	JZX	C12-N3-C9	2.49	114.30	108.90
2	A	1	JZX	O2-S2-N5	2.54	109.54	106.99
2	A	1	JZX	C8-C1-N1	2.63	121.55	116.31
2	A	1	JZX	C1-N1-C3	3.24	118.42	116.21
2	A	1	JZX	C2-N2-C1	3.40	122.55	116.38
2	A	1	JZX	C21-S2-N5	4.81	111.81	107.35
2	A	1	JZX	C5-C7-N3	5.88	124.24	113.00

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	1	JZX	2	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	841/966 (87%)	1.07	145 (17%) 2 1	11, 71, 109, 143	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	13.7
1	A	322	GLU	11.6
1	A	253	ALA	11.0
1	A	1086	TRP	9.9
1	A	376	ASN	8.6
1	A	267	GLU	7.7
1	A	216	ALA	6.9
1	A	143	MET	6.9
1	A	1088	LEU	6.8
1	A	896	VAL	6.6
1	A	823	LEU	6.2
1	A	378	ASP	6.2
1	A	374	PRO	6.1
1	A	321	GLU	5.6
1	A	268	GLN	5.5
1	A	1077	ASP	5.5
1	A	835	GLY	5.5
1	A	269	ASP	5.4
1	A	528	ALA	5.1
1	A	359	ARG	5.0
1	A	857	THR	5.0
1	A	824	SER	5.0
1	A	1046	GLU	5.0
1	A	895	THR	4.8
1	A	1075	CYS	4.8
1	A	756	LYS	4.6
1	A	1091	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	1043	THR	4.6
1	A	212	TRP	4.5
1	A	983	VAL	4.5
1	A	213	LYS	4.4
1	A	894	SER	4.4
1	A	916	PRO	4.3
1	A	375	ARG	4.3
1	A	148	GLN	4.3
1	A	757	TYR	4.1
1	A	612	ALA	4.1
1	A	252	MET	4.0
1	A	522	ASN	3.9
1	A	967	HIS	3.7
1	A	765	SER	3.7
1	A	270	PHE	3.7
1	A	1064	ALA	3.6
1	A	758	ASP	3.6
1	A	1089	HIS	3.5
1	A	762	GLN	3.5
1	A	163	THR	3.5
1	A	1045	LYS	3.5
1	A	1040	PRO	3.4
1	A	999	GLY	3.4
1	A	998	SER	3.4
1	A	1000	LYS	3.4
1	A	982	ARG	3.4
1	A	987	LEU	3.4
1	A	1070	ASP	3.4
1	A	751	SER	3.4
1	A	919	GLU	3.3
1	A	544	ARG	3.3
1	A	905	GLU	3.2
1	A	561	THR	3.2
1	A	748	ASP	3.2
1	A	613	ARG	3.2
1	A	898	ASN	3.1
1	A	251	LYS	3.1
1	A	435	CYS	3.1
1	A	1090	LEU	3.1
1	A	917	THR	3.1
1	A	806	SER	3.1
1	A	926	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	899	THR	3.0
1	A	166	SER	3.0
1	A	527	ILE	3.0
1	A	615	GLU	3.0
1	A	227	SER	3.0
1	A	1007	GLN	2.9
1	A	902	PHE	2.9
1	A	993	PHE	2.9
1	A	825	ASN	2.9
1	A	390	GLY	2.9
1	A	1076	ARG	2.8
1	A	238	ASP	2.8
1	A	809	LYS	2.7
1	A	521	ASP	2.7
1	A	149	ALA	2.7
1	A	513	SER	2.7
1	A	646	GLN	2.7
1	A	1084	PHE	2.7
1	A	1008	LYS	2.6
1	A	821	THR	2.6
1	A	988	THR	2.6
1	A	820	PRO	2.6
1	A	950	ASP	2.6
1	A	826	GLU	2.6
1	A	836	ASP	2.6
1	A	707	ARG	2.5
1	A	401	PRO	2.5
1	A	752	LEU	2.5
1	A	228	THR	2.5
1	A	377	THR	2.5
1	A	549	ASN	2.5
1	A	772	GLU	2.5
1	A	1082	VAL	2.4
1	A	210	TYR	2.4
1	A	250	THR	2.4
1	A	837	ASP	2.4
1	A	900	GLY	2.4
1	A	283	GLY	2.4
1	A	217	ASN	2.4
1	A	995	MET	2.3
1	A	545	ALA	2.3
1	A	1038	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	764	ILE	2.3
1	A	249	PHE	2.3
1	A	231	GLN	2.3
1	A	834	HIS	2.3
1	A	1048	ILE	2.2
1	A	920	LYS	2.2
1	A	877	GLY	2.2
1	A	893	GLN	2.2
1	A	888	ILE	2.2
1	A	873	GLY	2.2
1	A	243	ALA	2.2
1	A	358	ASP	2.2
1	A	930	TYR	2.2
1	A	460	LEU	2.2
1	A	409	LEU	2.2
1	A	874	ASP	2.1
1	A	786	PRO	2.1
1	A	147	SER	2.1
1	A	546	GLU	2.1
1	A	471	HIS	2.1
1	A	831	ILE	2.1
1	A	951	ASN	2.1
1	A	315	LEU	2.1
1	A	171	ASP	2.1
1	A	413	TRP	2.1
1	A	233	ILE	2.0
1	A	305	VAL	2.0
1	A	901	ALA	2.0
1	A	747	LEU	2.0
1	A	371	PRO	2.0
1	A	192	ASP	2.0
1	A	304	HIS	2.0
1	A	1011	ASP	2.0
1	A	892	GLN	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 [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( $\text{\AA}^2$ )	Q<0.9
2	JZX	A	1	33/33	0.90	0.33	1.20	44,47,70,71	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.