



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:23 AM GMT

PDB ID : 2WXL  
Title : THE CRYSTAL STRUCTURE OF THE MURINE CLASS IA PI 3-KINASE P110DELTA IN COMPLEX WITH ZSTK474.  
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 : 1.99 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

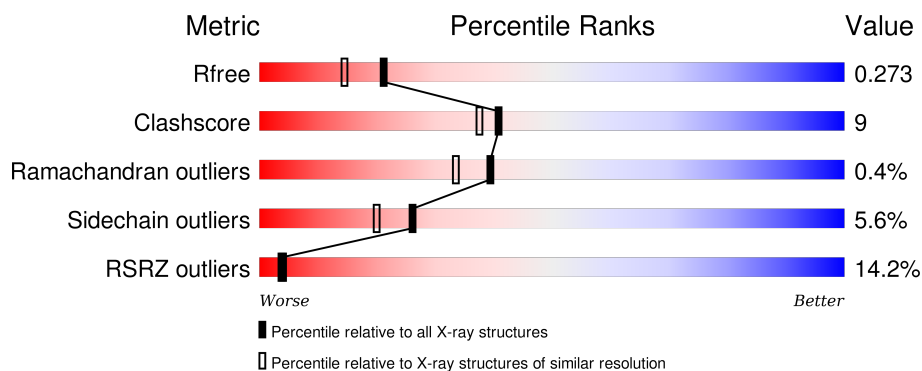
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6944 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.

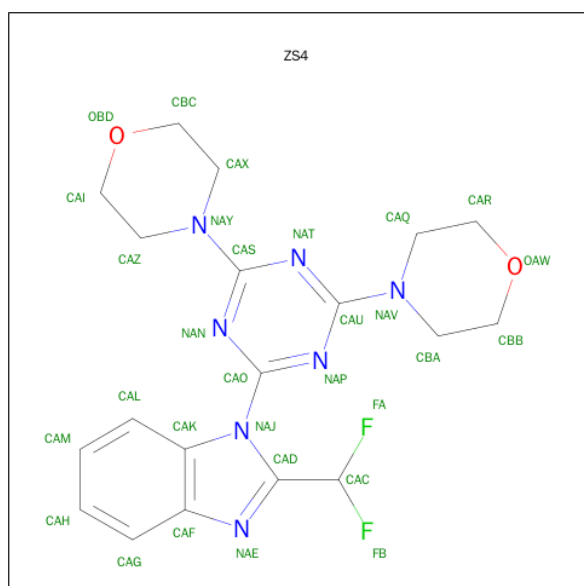
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	823	6656	4268	1131	1203	54	0	2	0

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-(DIFLUOROMETHYL)-1-(4,6-DIMORPHOLIN-4-YL-1,3,5-TRIAZIN-2-YL)-1H-BENZIMIDAZOLE (three-letter code: ZS4) (formula: C<sub>19</sub>H<sub>21</sub>F<sub>2</sub>N<sub>7</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	30	19	2	7	2	0	0

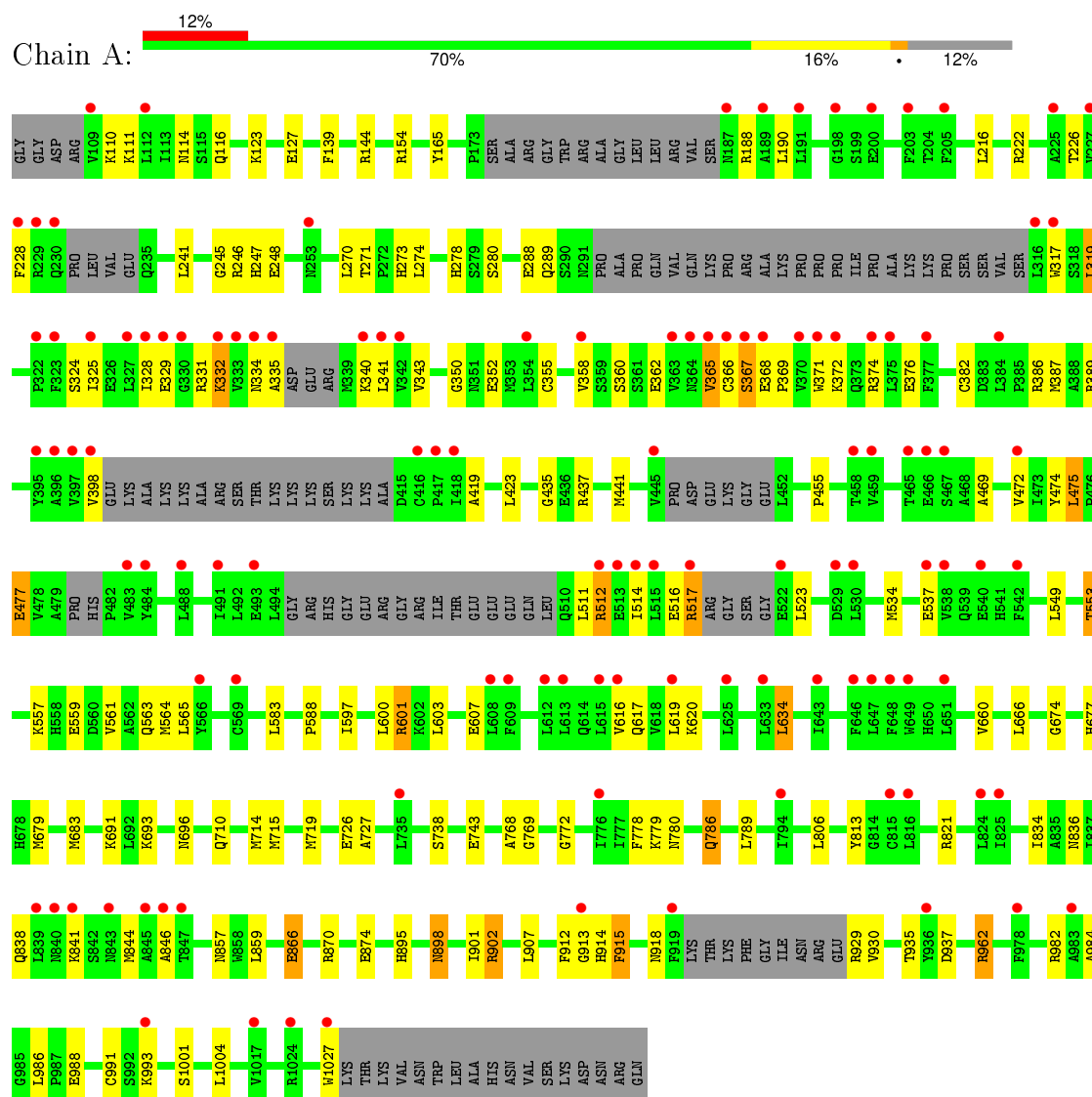
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	258	Total 258	O 258	0	0

### 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 DELTA ISOFORM



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.54Å 64.29Å 116.72Å 90.00° 103.42° 90.00°	Depositor
Resolution (Å)	37.85 – 1.99 37.84 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.85-1.99) 99.5 (37.84-1.99)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, $R_{free}$	0.214 , 0.254 0.239 , 0.273	Depositor DCC
$R_{free}$ test set	2115 reflections (3.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 70086 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: ZS4

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	0.62	4/6805 (0.1%)	0.67	3/9180 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	CYS	CB-SG	8.27	1.96	1.82
1	A	355	CYS	CB-SG	7.50	1.95	1.82
1	A	362	GLU	CD-OE2	5.49	1.31	1.25
1	A	813	TYR	CD1-CE1	5.30	1.47	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	902	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	A	902	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	634	LEU	CA-CB-CG	5.41	127.75	115.30

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	6656	0	6642	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	30	0	21	1	0
3	A	258	0	0	12	0
All	All	6944	0	6663	115	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 9.

All (115) 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:367:SER:HB3	1:A:368:GLU:C	1.70	1.12
1:A:549:LEU:HG	1:A:564:MET:HE1	1.26	1.09
1:A:962[A]:ARG:HH11	1:A:962[A]:ARG:HG2	1.19	1.07
1:A:962[A]:ARG:NH1	1:A:962[A]:ARG:HG2	1.74	0.98
1:A:962[A]:ARG:HH11	1:A:962[A]:ARG:CG	1.75	0.98
1:A:549:LEU:HG	1:A:564:MET:CE	2.02	0.88
1:A:110:LYS:HE3	1:A:114:ASN:HD21	1.38	0.87
1:A:902:ARG:HD3	3:A:2201:HOH:O	1.76	0.85
1:A:328:ILE:O	1:A:371:TRP:O	1.92	0.85
1:A:836:ASN:CG	3:A:2208:HOH:O	2.17	0.82
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.15	0.80
1:A:553:THR:CG2	1:A:564:MET:HE3	2.16	0.76
1:A:110:LYS:NZ	1:A:144:ARG:HH12	1.88	0.72
1:A:929:ARG:HH22	1:A:1001:SER:HB3	1.56	0.71
1:A:512:ARG:HH11	1:A:512:ARG:HG3	1.54	0.70
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.56	0.70
1:A:821:ARG:HD2	3:A:2193:HOH:O	1.91	0.70
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.73	0.70
1:A:902:ARG:CD	3:A:2201:HOH:O	2.34	0.69
1:A:553:THR:HG21	1:A:564:MET:HE3	1.75	0.67
1:A:512:ARG:O	1:A:516:GLU:HB2	1.97	0.65
1:A:278:HIS:HD2	1:A:280:SER:OG	1.80	0.63
1:A:768:ALA:HB3	1:A:772:GLY:HA3	1.78	0.63
1:A:386:ARG:HG3	1:A:387:MET:CE	2.28	0.63
1:A:806:LEU:HD13	1:A:962[B]:ARG:HD2	1.82	0.62
1:A:367:SER:HB3	1:A:368:GLU:CA	2.29	0.62
1:A:367:SER:HB3	1:A:368:GLU:O	2.00	0.61
1:A:222:ARG:O	1:A:226:THR:HG23	2.00	0.61
1:A:332:LYS:HZ2	1:A:341:LEU:HD21	1.65	0.61
1:A:620:LYS:HE2	1:A:660:VAL:HG11	1.82	0.60
1:A:332:LYS:HZ3	1:A:341:LEU:HD11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.84	0.60
1:A:123:LYS:NZ	1:A:127:GLU:OE1	2.36	0.59
1:A:836:ASN:HB2	3:A:2208:HOH:O	2.02	0.58
1:A:836:ASN:CB	3:A:2208:HOH:O	2.50	0.58
1:A:895:HIS:H	1:A:898:ASN:HD21	1.51	0.58
1:A:435:GLY:HA2	1:A:475:LEU:O	2.05	0.56
1:A:915:PHE:CD1	1:A:915:PHE:C	2.79	0.56
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.88	0.55
1:A:419:ALA:HB3	1:A:441:MET:HE1	1.87	0.55
1:A:870:ARG:NH2	1:A:874:GLU:OE2	2.40	0.55
1:A:512:ARG:NH1	1:A:534:MET:HG3	2.22	0.55
1:A:319:LEU:HD23	1:A:319:LEU:N	2.22	0.54
1:A:154:ARG:HH11	1:A:154:ARG:HG2	1.72	0.54
1:A:324:SER:HB3	1:A:376:GLU:HG3	1.90	0.54
1:A:841:LYS:HB2	1:A:844:MET:HG3	1.89	0.53
1:A:154:ARG:HD2	1:A:165:TYR:CE2	2.43	0.53
1:A:779:LYS:HG2	3:A:2166:HOH:O	2.08	0.52
1:A:389:ARG:NH1	1:A:455:PRO:O	2.40	0.52
1:A:216:LEU:HD22	1:A:241:LEU:HD11	1.92	0.51
1:A:110:LYS:HE3	1:A:114:ASN:ND2	2.19	0.51
1:A:329:GLU:HB2	1:A:369:PRO:O	2.11	0.51
1:A:617:GLN:NE2	1:A:984:ALA:HA	2.23	0.51
1:A:553:THR:CG2	1:A:564:MET:CE	2.88	0.50
1:A:371:TRP:O	1:A:372:LYS:HG3	2.10	0.50
1:A:914:HIS:HB3	1:A:918:ASN:O	2.12	0.50
1:A:786:GLN:HE22	1:A:988:GLU:HB2	1.77	0.50
1:A:929:ARG:HH22	1:A:1001:SER:CB	2.22	0.49
1:A:154:ARG:NH2	1:A:674:GLY:O	2.46	0.49
1:A:838:GLN:NE2	1:A:937:ASP:OD2	2.45	0.49
1:A:895:HIS:H	1:A:898:ASN:ND2	2.11	0.49
1:A:343:VAL:H	1:A:360:SER:HB3	1.78	0.49
1:A:915:PHE:HD1	1:A:915:PHE:C	2.16	0.48
1:A:366:CYS:O	1:A:367:SER:HB2	2.13	0.48
1:A:241:LEU:HD13	1:A:274:LEU:HD13	1.95	0.48
1:A:982:ARG:NH2	1:A:991:CYS:HA	2.29	0.47
1:A:715:MET:O	1:A:719:MET:HG3	2.15	0.47
1:A:617:GLN:HE21	1:A:984:ALA:CA	2.27	0.47
1:A:693:LYS:HE2	1:A:780:ASN:ND2	2.29	0.47
1:A:597:ILE:HG22	1:A:601:ARG:NH2	2.30	0.47
1:A:588:PRO:HD2	3:A:2077:HOH:O	2.14	0.47
1:A:332:LYS:NZ	1:A:341:LEU:HD11	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:HIS:O	1:A:738:SER:HB2	2.15	0.46
1:A:561:VAL:O	1:A:565:LEU:HD13	2.15	0.46
1:A:553:THR:HG22	1:A:564:MET:CE	2.46	0.46
1:A:154:ARG:HD2	1:A:165:TYR:CZ	2.51	0.46
1:A:913:GLY:N	3:A:2232:HOH:O	2.49	0.46
1:A:289:GLN:HG2	1:A:677:HIS:CD2	2.51	0.45
1:A:332:LYS:HZ1	1:A:334:ASN:HB3	1.82	0.45
1:A:328:ILE:HD11	1:A:474:TYR:HB2	1.97	0.45
1:A:907:LEU:C	1:A:907:LEU:HD23	2.38	0.45
2:A:1500:ZS4:NAN	2:A:1500:ZS4:CAC	2.80	0.44
1:A:691:LYS:HG3	1:A:727:ALA:CB	2.47	0.44
1:A:512:ARG:HG3	1:A:512:ARG:NH1	2.29	0.44
1:A:583:LEU:HD11	1:A:600:LEU:HD11	2.00	0.44
1:A:334:ASN:CG	1:A:335:ALA:H	2.21	0.44
1:A:334:ASN:HD22	1:A:365:VAL:HG22	1.83	0.44
1:A:834:ILE:O	1:A:838:GLN:HG3	2.18	0.44
1:A:859:LEU:HD21	1:A:901:ILE:HD11	1.98	0.44
1:A:350:GLY:HA3	1:A:588:PRO:HG3	2.00	0.43
1:A:603:LEU:HD22	1:A:607:GLU:HB3	2.00	0.43
1:A:477:GLU:HG2	1:A:477:GLU:H	1.53	0.43
1:A:419:ALA:HB3	1:A:441:MET:CE	2.48	0.43
1:A:537:GLU:HG3	3:A:2067:HOH:O	2.19	0.43
1:A:902:ARG:HD2	3:A:2201:HOH:O	2.11	0.43
1:A:334:ASN:CG	1:A:335:ALA:N	2.72	0.43
1:A:982:ARG:HH21	1:A:991:CYS:HA	1.83	0.43
1:A:912:PHE:HA	3:A:2232:HOH:O	2.18	0.43
1:A:516:GLU:C	1:A:517:ARG:HG2	2.39	0.42
1:A:343:VAL:H	1:A:360:SER:CB	2.32	0.42
1:A:139:PHE:CE2	1:A:666:LEU:HB3	2.54	0.42
1:A:866:GLU:HG2	1:A:866:GLU:H	1.36	0.42
1:A:693:LYS:HE2	1:A:780:ASN:HD21	1.84	0.42
1:A:846:ALA:HA	1:A:857:ASN:HB3	2.01	0.42
1:A:679:MET:O	1:A:683:MET:HG3	2.20	0.42
1:A:331:ARG:O	1:A:469:ALA:HA	2.19	0.41
1:A:789:LEU:HD23	1:A:915:PHE:CE2	2.56	0.41
1:A:288:GLU:HG2	1:A:289:GLN:HG3	2.02	0.41
1:A:325:ILE:HG22	1:A:475:LEU:HD12	2.03	0.41
1:A:271:THR:O	1:A:273:HIS:HD2	2.03	0.40
1:A:616:VAL:O	1:A:619:LEU:HB2	2.21	0.40
1:A:696:ASN:HD22	1:A:778:PHE:HD2	1.69	0.40
1:A:710:GLN:O	1:A:714:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:SER:HB3	1:A:369:PRO:N	2.30	0.40
1:A:116:GLN:HB3	1:A:683:MET:SD	2.62	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	803/940 (85%)	777 (97%)	23 (3%)	3 (0%)	39 33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	SER
1	A	365	VAL
1	A	769	GLY

### 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	731/827 (88%)	689 (94%)	42 (6%)	25 19

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	228	PHE
1	A	270	LEU
1	A	317	TRP
1	A	319	LEU
1	A	332	LYS
1	A	340	LYS
1	A	352	GLU
1	A	358	VAL
1	A	374	ARG
1	A	398	VAL
1	A	423	LEU
1	A	437	ARG
1	A	475	LEU
1	A	477	GLU
1	A	511	LEU
1	A	512	ARG
1	A	514	ILE
1	A	517	ARG
1	A	523	LEU
1	A	553	THR
1	A	557	LYS
1	A	559	GLU
1	A	563	GLN
1	A	601	ARG
1	A	634	LEU
1	A	726	GLU
1	A	743	GLU
1	A	786	GLN
1	A	866	GLU
1	A	898	ASN
1	A	915	PHE
1	A	930	VAL
1	A	935	THR
1	A	962[A]	ARG
1	A	962[B]	ARG
1	A	986	LEU
1	A	993	LYS
1	A	1004	LEU
1	A	1027	TRP

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	116	GLN
1	A	273	HIS
1	A	278	HIS
1	A	334	ASN
1	A	431	GLN
1	A	563	GLN
1	A	617	GLN
1	A	780	ASN
1	A	786	GLN
1	A	838	GLN
1	A	898	ASN
1	A	906	GLN
1	A	918	ASN
1	A	943	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	ZS4	A	1500	-	30,34,34	1.52	4 (13%)	36,48,48	2.22	12 (33%)

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	ZS4	A	1500	-	-	0/8/32/32	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	ZS4	CAK-NAJ	-5.25	1.32	1.39
2	A	1500	ZS4	CAD-NAJ	-2.65	1.33	1.37
2	A	1500	ZS4	CAS-NAY	2.10	1.39	1.35
2	A	1500	ZS4	CAU-NAV	2.45	1.40	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	ZS4	NAT-CAU-NAP	-4.02	119.58	126.35
2	A	1500	ZS4	NAN-CAO-NAP	-3.81	119.83	126.37
2	A	1500	ZS4	NAN-CAS-NAT	-3.02	121.27	126.35
2	A	1500	ZS4	OBD-CAI-CAZ	2.03	116.48	111.84
2	A	1500	ZS4	CBA-NAV-CAQ	2.57	116.98	111.59
2	A	1500	ZS4	NAN-CAS-NAY	2.73	120.14	117.08
2	A	1500	ZS4	CAO-NAN-CAS	3.34	118.86	113.48
2	A	1500	ZS4	CAS-NAT-CAU	3.51	119.14	113.48
2	A	1500	ZS4	NAP-CAU-NAV	3.79	121.33	117.08
2	A	1500	ZS4	CAX-NAY-CAZ	4.30	120.61	111.59
2	A	1500	ZS4	CBC-OBD-CAI	4.46	124.92	109.89
2	A	1500	ZS4	CAO-NAP-CAU	4.84	121.27	113.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	ZS4	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	823/940 (87%)	0.92	117 (14%) 4 4	2, 14, 28, 49	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	CYS	7.9
1	A	846	ALA	7.8
1	A	514	ILE	7.8
1	A	445	VAL	6.6
1	A	919	PHE	6.6
1	A	334	ASN	6.3
1	A	363	VAL	6.2
1	A	330	GLY	5.8
1	A	488	LEU	5.7
1	A	228	PHE	5.7
1	A	341	LEU	5.5
1	A	205	PHE	5.3
1	A	847	THR	5.2
1	A	395	TYR	4.9
1	A	370	VAL	4.9
1	A	317	TRP	4.5
1	A	416	CYS	4.3
1	A	522	GLU	4.2
1	A	839	LEU	4.1
1	A	367	SER	3.9
1	A	616	VAL	3.8
1	A	467	SER	3.8
1	A	364	ASN	3.8
1	A	397	VAL	3.8
1	A	377	PHE	3.7
1	A	1027	TRP	3.7
1	A	365	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	619	LEU	3.7
1	A	542	PHE	3.7
1	A	340	LYS	3.7
1	A	466	GLU	3.7
1	A	515	LEU	3.6
1	A	371	TRP	3.5
1	A	613	LEU	3.5
1	A	329	GLU	3.5
1	A	396	ALA	3.4
1	A	612	LEU	3.4
1	A	512	ARG	3.3
1	A	398	VAL	3.3
1	A	529	ASP	3.3
1	A	615	LEU	3.2
1	A	230	GLN	3.2
1	A	472	VAL	3.2
1	A	651	LEU	3.2
1	A	203	PHE	3.2
1	A	841	LYS	3.1
1	A	191	LEU	3.1
1	A	322	PRO	3.1
1	A	493	GLU	3.1
1	A	372	LYS	3.0
1	A	735	LEU	3.0
1	A	936	TYR	3.0
1	A	342	VAL	3.0
1	A	332	LYS	3.0
1	A	459	VAL	3.0
1	A	816	LEU	2.9
1	A	643	ILE	2.9
1	A	491	ILE	2.9
1	A	633	LEU	2.8
1	A	187	ASN	2.8
1	A	843	ASN	2.8
1	A	609	PHE	2.8
1	A	325	ILE	2.7
1	A	537	GLU	2.7
1	A	189	ALA	2.7
1	A	375	LEU	2.7
1	A	198	GLY	2.7
1	A	647	LEU	2.6
1	A	225	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	323	PHE	2.6
1	A	824	LEU	2.5
1	A	993	LYS	2.5
1	A	227	VAL	2.5
1	A	358	VAL	2.5
1	A	845	ALA	2.5
1	A	418	ILE	2.5
1	A	840	ASN	2.5
1	A	815	CYS	2.4
1	A	109	VAL	2.4
1	A	648	PHE	2.4
1	A	253	ASN	2.4
1	A	333	VAL	2.4
1	A	776	ILE	2.4
1	A	112	LEU	2.3
1	A	327	LEU	2.3
1	A	354	LEU	2.3
1	A	368	GLU	2.3
1	A	517	ARG	2.3
1	A	566	TYR	2.3
1	A	484	TYR	2.3
1	A	328	ILE	2.2
1	A	335	ALA	2.2
1	A	458	THR	2.2
1	A	465	THR	2.2
1	A	649	TRP	2.2
1	A	530	LEU	2.2
1	A	625	LEU	2.2
1	A	513	GLU	2.2
1	A	483	VAL	2.2
1	A	316	LEU	2.2
1	A	374	ARG	2.1
1	A	794	ILE	2.1
1	A	1024	ARG	2.1
1	A	913	GLY	2.1
1	A	417	PRO	2.1
1	A	646	PHE	2.1
1	A	569	CYS	2.1
1	A	200	GLU	2.1
1	A	229	ARG	2.1
1	A	983	ALA	2.0
1	A	608	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	538	VAL	2.0
1	A	1017	VAL	2.0
1	A	540	GLU	2.0
1	A	825	ILE	2.0
1	A	978	PHE	2.0
1	A	384	LEU	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( $\text{\AA}^2$ )	Q<0.9
2	ZS4	A	1500	30/30	0.96	0.12	-0.29	19,26,34,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.