



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:23 AM GMT

PDB ID : 2WXH  
Title : THE CRYSTAL STRUCTURE OF THE MURINE CLASS IA PI 3-KINASE P110DELTA IN COMPLEX WITH SW14.  
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

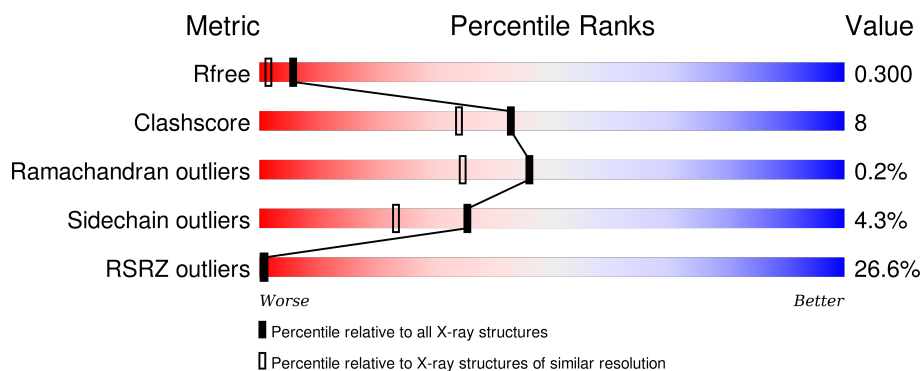
# 1 Overall quality at a glance

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>23%</div> <div>71%</div> <div>16%</div> <div>13%</div> </div>

## 2 Entry composition [i](#)

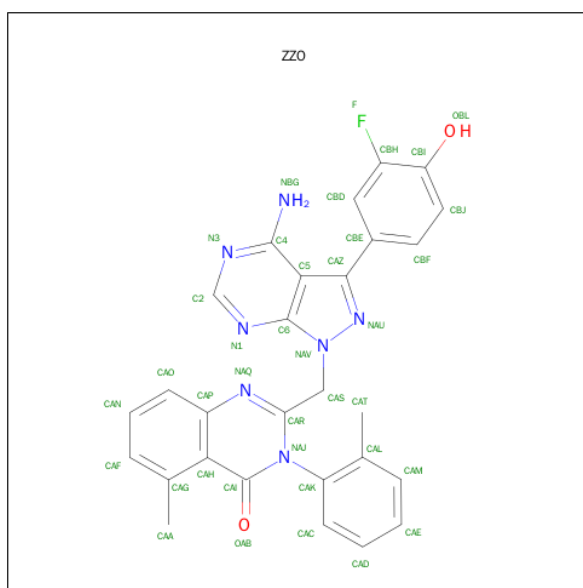
There are 3 unique types of molecules in this entry. The entry contains 6949 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	0	0
			6633	4254	1126	1199	54			

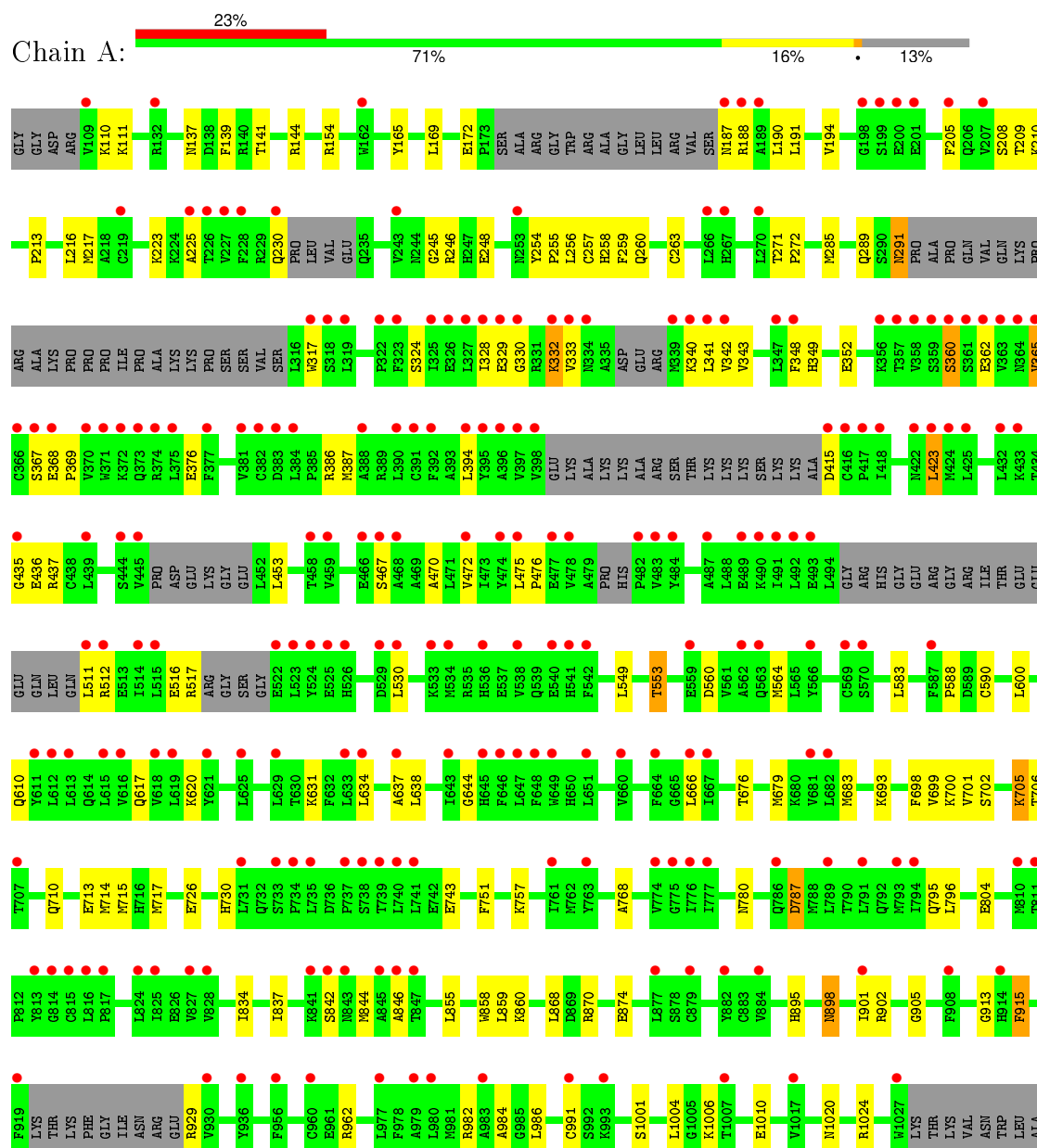
- Molecule 2 is 2-{[4-AMINO-3-(3-FLUORO-4-HYDROXYPHENYL)-1H-PYRAZOLO[3,4-D]PYRIMIDIN-1-YL]METHYL}-5-METHYL-3-(2-METHYLPHENYL)QUINAZOLIN-4(3H)-ONE (three-letter code: ZZO) (formula: C<sub>28</sub>H<sub>22</sub>FN<sub>7</sub>O<sub>2</sub>).



### 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



HIS
ASN
VAL
SER
LYS
ASP
ASN
ARG
GLN

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.87Å 65.01Å 117.08Å 90.00° 103.58° 90.00°	Depositor
Resolution (Å)	38.04 – 1.90 37.94 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.04-1.90) 99.2 (37.94-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0053	Depositor
R, $R_{free}$	0.217 , 0.245 0.276 , 0.300	Depositor DCC
$R_{free}$ test set	2480 reflections (3.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.3	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 81811 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	7.0	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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.54	0/6776	0.63	3/9142 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	902	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	A	902	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	423	LEU	CA-CB-CG	5.13	127.10	115.30

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	6633	0	6615	109	0
2	A	38	0	21	1	0
3	A	278	0	0	2	0
All	All	6949	0	6636	109	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 8.

All (109) 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	1.78	1.02
1:A:837:ILE:HD11	1:A:901:ILE:HD11	1.46	0.96
1:A:837:ILE:CD1	1:A:901:ILE:HD11	2.03	0.89
1:A:901:ILE:O	1:A:901:ILE:HD12	1.77	0.85
1:A:706:THR:OG1	1:A:710:GLN:OE1	1.98	0.81
1:A:846:ALA:HB1	3:A:2222:HOH:O	1.80	0.81
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.66	0.76
1:A:699:VAL:HG21	1:A:715:MET:HE2	1.66	0.76
1:A:549:LEU:HG	1:A:564:MET:CE	2.16	0.75
1:A:715:MET:HE1	1:A:751:PHE:HB3	1.69	0.75
1:A:962:ARG:HG2	1:A:962:ARG:HH11	1.52	0.75
1:A:895:HIS:H	1:A:898:ASN:HD21	1.38	0.72
1:A:332:LYS:NZ	1:A:341:LEU:HD21	2.04	0.71
1:A:787:ASP:OD2	2:A:1500:ZZO:OBL	2.09	0.71
1:A:858:TRP:CZ3	1:A:901:ILE:HD13	2.26	0.70
1:A:332:LYS:HZ2	1:A:341:LEU:HD21	1.57	0.70
1:A:365:VAL:HG12	1:A:365:VAL:O	1.91	0.69
1:A:367:SER:HB3	1:A:368:GLU:CA	2.21	0.69
1:A:553:THR:HG21	1:A:564:MET:HE2	1.74	0.69
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.73	0.69
1:A:699:VAL:HG21	1:A:715:MET:CE	2.24	0.68
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.77	0.67
1:A:549:LEU:HG	1:A:564:MET:HE3	1.75	0.66
1:A:365:VAL:CG1	1:A:365:VAL:O	2.44	0.66
1:A:553:THR:CG2	1:A:564:MET:HE2	2.26	0.64
1:A:205:PHE:CE1	1:A:223:LYS:HG3	2.34	0.63
1:A:367:SER:HB3	1:A:368:GLU:O	1.99	0.62
1:A:435:GLY:HA2	1:A:475:LEU:O	2.01	0.60
1:A:329:GLU:HB2	1:A:369:PRO:O	2.02	0.60
1:A:834:ILE:HD11	1:A:901:ILE:HG23	1.83	0.60
1:A:929:ARG:HH22	1:A:1001:SER:HB3	1.67	0.59
1:A:549:LEU:HG	1:A:564:MET:HE1	1.83	0.59
1:A:870:ARG:NH2	1:A:874:GLU:OE2	2.34	0.59
1:A:929:ARG:HH22	1:A:1001:SER:CB	2.16	0.57
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.69	0.57
1:A:701:VAL:O	1:A:705:LYS:HD2	2.03	0.57
1:A:679:MET:O	1:A:683:MET:HG3	2.04	0.57
1:A:332:LYS:HE3	1:A:333:VAL:N	2.20	0.57
1:A:842:SER:O	1:A:844:MET:HG2	2.04	0.56
1:A:110:LYS:NZ	1:A:144:ARG:HH12	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LYS:HD2	1:A:341:LEU:HD11	1.90	0.53
1:A:329:GLU:HG2	1:A:472:VAL:CG2	2.38	0.53
1:A:553:THR:HG21	1:A:564:MET:CE	2.37	0.53
1:A:984:ALA:HB3	1:A:986:LEU:HD13	1.90	0.53
1:A:110:LYS:HZ1	1:A:144:ARG:HH12	1.56	0.53
1:A:915:PHE:CD2	1:A:915:PHE:C	2.83	0.52
1:A:342:VAL:HG22	1:A:362:GLU:HG2	1.91	0.52
1:A:436:GLU:O	1:A:437:ARG:HD2	2.09	0.52
1:A:895:HIS:H	1:A:898:ASN:ND2	2.06	0.52
1:A:154:ARG:HD2	1:A:165:TYR:CE2	2.44	0.52
1:A:553:THR:CG2	1:A:564:MET:CE	2.88	0.52
1:A:512:ARG:O	1:A:516:GLU:HB2	2.10	0.51
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.44	0.51
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.92	0.51
1:A:693:LYS:HE2	1:A:780:ASN:ND2	2.27	0.49
1:A:1020:ASN:O	1:A:1024:ARG:HG3	2.13	0.49
1:A:860:LYS:HG2	1:A:868:LEU:HD22	1.96	0.47
1:A:213:PRO:O	1:A:217:MET:HG3	2.14	0.47
1:A:617:GLN:HE22	1:A:620:LYS:NZ	2.12	0.47
1:A:859:LEU:HD21	1:A:905:GLY:HA2	1.95	0.47
1:A:583:LEU:HD11	1:A:600:LEU:CD1	2.45	0.46
1:A:343:VAL:H	1:A:360:SER:HB2	1.78	0.46
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.80	0.46
1:A:187:ASN:N	1:A:210:LYS:HZ2	2.11	0.46
1:A:225:ALA:O	1:A:230:GLN:N	2.49	0.46
1:A:205:PHE:HE1	1:A:223:LYS:HG3	1.78	0.46
1:A:194:VAL:HG21	1:A:216:LEU:CD2	2.45	0.46
1:A:216:LEU:HD12	1:A:256:LEU:HD11	1.98	0.45
1:A:437:ARG:O	1:A:472:VAL:HA	2.15	0.45
1:A:698:PHE:HZ	1:A:714:MET:HB3	1.81	0.45
1:A:348:PHE:HE2	1:A:453:LEU:HD23	1.81	0.45
1:A:617:GLN:HE22	1:A:620:LYS:HZ2	1.64	0.45
1:A:172:GLU:OE1	1:A:260:GLN:HG2	2.17	0.44
1:A:982:ARG:NH2	1:A:991:CYS:HA	2.33	0.44
1:A:962:ARG:CG	1:A:962:ARG:HH11	2.28	0.43
1:A:194:VAL:CG2	1:A:216:LEU:HD21	2.45	0.43
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.99	0.43
1:A:213:PRO:HD3	1:A:254:TYR:O	2.18	0.43
1:A:137:ASN:O	1:A:141:THR:HG23	2.18	0.43
1:A:332:LYS:HZ3	1:A:341:LEU:HD21	1.82	0.43
1:A:285:MET:O	1:A:289:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PRO:HG2	1:A:258:HIS:CD2	2.53	0.43
1:A:698:PHE:CZ	1:A:714:MET:HB3	2.54	0.42
1:A:475:LEU:HA	1:A:476:PRO:HD3	1.89	0.42
1:A:858:TRP:CH2	1:A:901:ILE:HD13	2.54	0.42
1:A:1006:LYS:HB3	1:A:1010:GLU:HB2	2.00	0.42
1:A:387:MET:HE2	1:A:590:CYS:SG	2.59	0.42
1:A:349:HIS:NE2	1:A:588:PRO:HG2	2.35	0.42
1:A:208:SER:OG	1:A:210:LYS:HG2	2.19	0.42
1:A:169:LEU:HD22	1:A:259:PHE:HE1	1.85	0.42
1:A:730:HIS:HD2	3:A:2139:HOH:O	2.03	0.42
1:A:693:LYS:HE2	1:A:780:ASN:HD21	1.85	0.41
1:A:348:PHE:CE2	1:A:453:LEU:HD23	2.54	0.41
1:A:637:ALA:HB1	1:A:644:GLY:HA2	2.02	0.41
1:A:386:ARG:HG3	1:A:387:MET:CE	2.51	0.41
1:A:209:THR:HB	1:A:257:CYS:HB3	2.02	0.41
1:A:139:PHE:CE2	1:A:666:LEU:HB3	2.54	0.41
1:A:610:GLN:HG2	1:A:796:LEU:HD13	2.02	0.41
1:A:713:GLU:O	1:A:717:MET:HG3	2.20	0.41
1:A:291:ASN:ND2	1:A:676:THR:H	2.19	0.41
1:A:702:SER:O	1:A:706:THR:HG22	2.21	0.41
1:A:329:GLU:HG2	1:A:472:VAL:HG22	2.03	0.41
1:A:191:LEU:O	1:A:271:THR:HG23	2.21	0.41
1:A:330:GLY:HA2	1:A:470:ALA:O	2.20	0.41
1:A:191:LEU:O	1:A:272:PRO:HD2	2.21	0.40
1:A:324:SER:HB3	1:A:376:GLU:HG3	2.03	0.40
1:A:700:LYS:HG2	1:A:757:LYS:HD2	2.04	0.40
1:A:154:ARG:HD2	1:A:165:TYR:CZ	2.56	0.40
1:A:638:LEU:HA	1:A:638:LEU:HD23	1.99	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	800/940 (85%)	775 (97%)	23 (3%)	2 (0%)	46 35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	VAL
1	A	913	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	728/827 (88%)	697 (96%)	31 (4%)	35 23

All (31) 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	263	CYS
1	A	291	ASN
1	A	317	TRP
1	A	332	LYS
1	A	340	LYS
1	A	352	GLU
1	A	360	SER
1	A	394	LEU
1	A	415	ASP
1	A	423	LEU
1	A	467	SER
1	A	511	LEU
1	A	517	ARG
1	A	530	LEU
1	A	553	THR
1	A	560	ASP

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Mol	Chain	Res	Type
1	A	631	LYS
1	A	634	LEU
1	A	705	LYS
1	A	726	GLU
1	A	743	GLU
1	A	787	ASP
1	A	795	GLN
1	A	804	GLU
1	A	855	LEU
1	A	898	ASN
1	A	915	PHE
1	A	1004	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	126	HIS
1	A	156	GLN
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	334	ASN
1	A	344	GLN
1	A	617	GLN
1	A	730	HIS
1	A	780	ASN
1	A	851	ASN
1	A	895	HIS
1	A	898	ASN
1	A	976	HIS

### 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	ZZO	A	1500	-	39,43,43	1.77	4 (10%)	37,64,64	2.88	10 (27%)

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	ZZO	A	1500	-	-	0/12/12/12	0/6/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	ZZO	CBE-CAZ	-7.21	1.40	1.49
2	A	1500	ZZO	CAK-NAJ	-3.30	1.41	1.45
2	A	1500	ZZO	CAA-CAG	2.19	1.55	1.51
2	A	1500	ZZO	CAS-CAR	4.90	1.54	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	ZZO	N1-C2-N3	-14.05	118.14	128.89
2	A	1500	ZZO	CBF-CBJ-CBI	-4.11	116.27	120.49
2	A	1500	ZZO	CBD-CBH-CBI	-4.02	120.49	123.78
2	A	1500	ZZO	CBE-CBD-CBH	-2.80	117.25	119.46
2	A	1500	ZZO	CBD-CBE-CAZ	-2.76	115.63	120.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	ZZO	CBF-CBE-CAZ	2.19	124.22	120.70
2	A	1500	ZZO	F-CBH-CBD	2.19	122.72	118.59
2	A	1500	ZZO	CAM-CAL-CAK	2.45	119.95	116.13
2	A	1500	ZZO	CAS-CAR-NAQ	2.53	119.71	116.09
2	A	1500	ZZO	C2-N3-C4	3.46	124.95	118.77

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	ZZO	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	822/940 (87%)	1.44	219 (26%) <b>1</b> <b>1</b>	2, 6, 19, 37	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	919	PHE	9.5
1	A	330	GLY	7.8
1	A	365	VAL	7.8
1	A	493	GLU	7.4
1	A	228	PHE	7.3
1	A	341	LEU	7.3
1	A	511	LEU	6.4
1	A	317	TRP	6.3
1	A	529	ASP	6.3
1	A	334	ASN	6.0
1	A	395	TYR	6.0
1	A	398	VAL	6.0
1	A	484	TYR	6.0
1	A	363	VAL	5.9
1	A	396	ALA	5.6
1	A	364	ASN	5.5
1	A	340	LYS	5.4
1	A	366	CYS	5.3
1	A	1027	TRP	5.3
1	A	227	VAL	5.2
1	A	514	ILE	5.2
1	A	377	PHE	5.1
1	A	445	VAL	5.1
1	A	333	VAL	5.0
1	A	735	LEU	4.9
1	A	397	VAL	4.7
1	A	417	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	416	CYS	4.7
1	A	846	ALA	4.6
1	A	542	PHE	4.6
1	A	342	VAL	4.6
1	A	332	LYS	4.6
1	A	843	ASN	4.4
1	A	373	GLN	4.4
1	A	526	HIS	4.4
1	A	847	THR	4.3
1	A	339	MET	4.3
1	A	492	LEU	4.2
1	A	776	ILE	4.2
1	A	482	PRO	4.2
1	A	619	LEU	4.1
1	A	187	ASN	4.1
1	A	390	LEU	4.0
1	A	459	VAL	4.0
1	A	541	HIS	4.0
1	A	522	GLU	3.9
1	A	824	LEU	3.9
1	A	467	SER	3.9
1	A	525	GLU	3.8
1	A	226	THR	3.7
1	A	201	GLU	3.7
1	A	367	SER	3.7
1	A	845	ALA	3.7
1	A	533	LYS	3.7
1	A	323	PHE	3.7
1	A	375	LEU	3.6
1	A	991	CYS	3.6
1	A	188	ARG	3.5
1	A	816	LEU	3.5
1	A	415	ASP	3.5
1	A	466	GLU	3.5
1	A	225	ALA	3.5
1	A	322	PRO	3.4
1	A	651	LEU	3.4
1	A	372	LYS	3.4
1	A	319	LEU	3.4
1	A	566	TYR	3.4
1	A	266	LEU	3.4
1	A	618	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	327	LEU	3.3
1	A	613	LEU	3.3
1	A	489	GLU	3.3
1	A	433	LYS	3.3
1	A	741	LEU	3.3
1	A	570	SER	3.3
1	A	356	LYS	3.3
1	A	360	SER	3.3
1	A	825	ILE	3.3
1	A	423	LEU	3.3
1	A	432	LEU	3.3
1	A	646	PHE	3.2
1	A	980	LEU	3.2
1	A	384	LEU	3.2
1	A	524	TYR	3.2
1	A	530	LEU	3.2
1	A	458	THR	3.1
1	A	648	PHE	3.1
1	A	189	ALA	3.1
1	A	794	ILE	3.1
1	A	647	LEU	3.1
1	A	329	GLU	3.1
1	A	512	ARG	3.1
1	A	534	MET	3.1
1	A	827	VAL	3.1
1	A	361	SER	3.1
1	A	612	LEU	3.1
1	A	815	CYS	3.1
1	A	739	THR	3.0
1	A	828	VAL	3.0
1	A	230	GLN	3.0
1	A	444	SER	2.9
1	A	777	ILE	2.9
1	A	198	GLY	2.9
1	A	616	VAL	2.9
1	A	774	VAL	2.9
1	A	325	ILE	2.9
1	A	814	GLY	2.9
1	A	625	LEU	2.9
1	A	813	TYR	2.9
1	A	908	PHE	2.8
1	A	789	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	381	VAL	2.8
1	A	477	GLU	2.8
1	A	523	LEU	2.8
1	A	358	VAL	2.8
1	A	842	SER	2.8
1	A	643	ILE	2.8
1	A	490	LYS	2.8
1	A	207	VAL	2.8
1	A	347	LEU	2.7
1	A	348	PHE	2.7
1	A	270	LEU	2.7
1	A	993	LYS	2.7
1	A	370	VAL	2.7
1	A	538	VAL	2.7
1	A	318	SER	2.7
1	A	649	TRP	2.7
1	A	761	ILE	2.7
1	A	132	ARG	2.7
1	A	487	ALA	2.7
1	A	243	VAL	2.6
1	A	391	CYS	2.6
1	A	569	CYS	2.6
1	A	763	TYR	2.6
1	A	326	GLU	2.6
1	A	515	LEU	2.6
1	A	109	VAL	2.6
1	A	200	GLU	2.6
1	A	667	ILE	2.6
1	A	205	PHE	2.6
1	A	615	LEU	2.6
1	A	681	VAL	2.6
1	A	738	SER	2.6
1	A	936	TYR	2.6
1	A	388	ALA	2.5
1	A	267	HIS	2.5
1	A	328	ILE	2.5
1	A	791	LEU	2.5
1	A	468	ALA	2.5
1	A	425	LEU	2.5
1	A	483	VAL	2.5
1	A	811	THR	2.5
1	A	1007	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	472	VAL	2.4
1	A	359	SER	2.4
1	A	901	ILE	2.4
1	A	563	GLN	2.4
1	A	731	LEU	2.4
1	A	362	GLU	2.4
1	A	775	GLY	2.4
1	A	645	HIS	2.4
1	A	424	MET	2.4
1	A	793	MET	2.4
1	A	199	SER	2.4
1	A	474	TYR	2.4
1	A	540	GLU	2.4
1	A	562	ALA	2.4
1	A	734	PRO	2.4
1	A	733	SER	2.4
1	A	491	ILE	2.3
1	A	219	CYS	2.3
1	A	439	LEU	2.3
1	A	877	LEU	2.3
1	A	884	VAL	2.3
1	A	637	ALA	2.3
1	A	740	LEU	2.3
1	A	664	PHE	2.3
1	A	621	TYR	2.3
1	A	435	GLY	2.3
1	A	682	LEU	2.3
1	A	977	LEU	2.3
1	A	368	GLU	2.2
1	A	382	CYS	2.2
1	A	418	ILE	2.2
1	A	882	TYR	2.2
1	A	559	GLU	2.2
1	A	374	ARG	2.2
1	A	914	HIS	2.2
1	A	633	LEU	2.2
1	A	634	LEU	2.2
1	A	979	ALA	2.1
1	A	536	HIS	2.1
1	A	629	LEU	2.1
1	A	666	LEU	2.1
1	A	1017	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	810	MET	2.1
1	A	475	LEU	2.1
1	A	162	TRP	2.1
1	A	371	TRP	2.1
1	A	392	PHE	2.1
1	A	956	PHE	2.1
1	A	660	VAL	2.1
1	A	422	ASN	2.1
1	A	841	LYS	2.1
1	A	983	ALA	2.1
1	A	478	VAL	2.1
1	A	930	VAL	2.1
1	A	786	GLN	2.1
1	A	587	PHE	2.0
1	A	611	TYR	2.0
1	A	960	CYS	2.0
1	A	707	THR	2.0
1	A	383	ASP	2.0
1	A	737	PRO	2.0
1	A	817	PRO	2.0
1	A	394	LEU	2.0
1	A	357	THR	2.0
1	A	253	ASN	2.0
1	A	879	CYS	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	ZZO	A	1500	38/38	0.93	0.11	-1.22	13,21,29,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.