



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:23 AM GMT

PDB ID : 2WXN  
Title : THE CRYSTAL STRUCTURE OF THE MURINE CLASS IA PI 3-KINASE P110DELTA IN COMPLEX WITH DL07.  
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Deposited on : 2009-11-09  
Resolution : 2.60 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

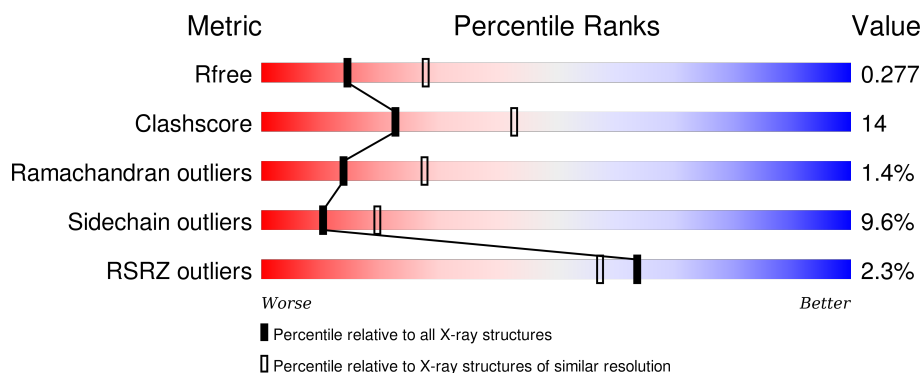
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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>2%</div> <div>59%</div> <div>25%</div> <div>•</div> <div>13%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6666 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.

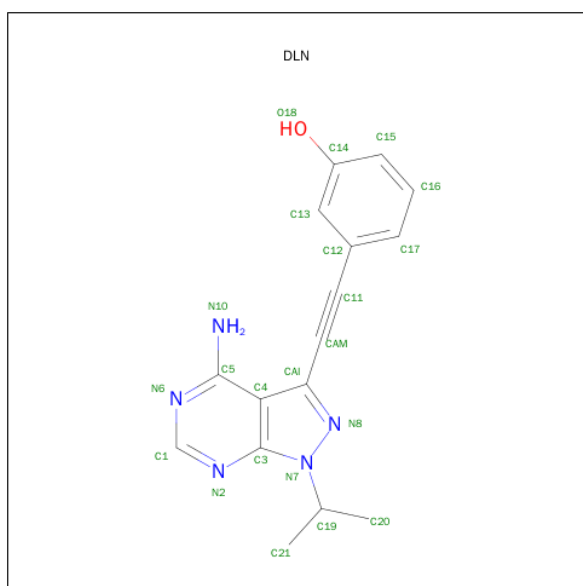
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	0	0
			6633	4254	1126	1199	54			

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 3-{[4-AMINO-1-(1-METHYLETHYL)-1H-PYRAZOLO[3,4-D]PYRIMIDIN-3-YL]ETHYNYL}PHENOL (three-letter code: DLN) (formula: C<sub>16</sub>H<sub>15</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			22	16	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.42Å 64.63Å 117.50Å 90.00° 103.43° 90.00°	Depositor
Resolution (Å)	57.17 – 2.60 39.06 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.9 (57.17-2.60) 91.9 (39.06-2.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, $R_{free}$	0.212 , 0.279 0.213 , 0.277	Depositor DCC
$R_{free}$ test set	921 reflections (3.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 58.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 29865 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6666	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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: DLN

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	0.79	2/6776 (0.0%)	0.84	4/9142 (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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	718	CYS	CB-SG	-6.77	1.70	1.82
1	A	745	CYS	CB-SG	-5.70	1.72	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	798	ASP	CB-CG-OD1	8.01	125.51	118.30
1	A	423	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	697	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	902	ARG	NE-CZ-NH2	-5.76	117.42	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	366	CYS	Peptide

## 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	6633	0	6615	179	0
2	A	22	0	15	5	0
3	A	11	0	0	1	0
All	All	6666	0	6630	180	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 14.

All (180) 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:332:LYS:H	1:A:332:LYS:HD3	1.07	1.12
1:A:367:SER:HB2	1:A:368:GLU:C	1.79	1.03
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.42	1.00
1:A:218:ALA:O	1:A:222:ARG:HG3	1.72	0.88
1:A:962:ARG:HG2	1:A:962:ARG:HH11	1.40	0.86
1:A:332:LYS:CD	1:A:332:LYS:H	1.89	0.83
1:A:617:GLN:NE2	1:A:984:ALA:HA	1.93	0.83
1:A:110:LYS:NZ	1:A:144:ARG:HH12	1.78	0.80
1:A:339:MET:O	1:A:365:VAL:HB	1.84	0.78
1:A:367:SER:HB3	1:A:368:GLU:HB3	1.64	0.78
1:A:332:LYS:HD3	1:A:332:LYS:N	1.91	0.75
1:A:367:SER:HB2	1:A:369:PRO:N	2.00	0.75
1:A:754:SER:O	1:A:757:LYS:HD3	1.87	0.74
1:A:110:LYS:HE3	1:A:114:ASN:HD21	1.55	0.71
1:A:284:ALA:O	1:A:288:GLU:HG3	1.90	0.71
1:A:700:LYS:NZ	1:A:780:ASN:HD22	1.90	0.70
1:A:855:LEU:O	1:A:855:LEU:HD23	1.91	0.70
1:A:345:ALA:O	1:A:357:THR:HB	1.92	0.70
1:A:799:VAL:O	1:A:803:GLN:HG3	1.92	0.69
1:A:205:PHE:HZ	1:A:223:LYS:HB2	1.59	0.68
1:A:553:THR:HG22	1:A:564:MET:HE3	1.76	0.68
1:A:512:ARG:HD3	1:A:534:MET:HG3	1.75	0.67
1:A:962:ARG:HG2	1:A:962:ARG:NH1	2.02	0.67
1:A:278:HIS:HD2	1:A:280:SER:OG	1.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:HD11	1:A:375:LEU:HD12	1.77	0.65
1:A:912:PHE:HA	3:A:2007:HOH:O	1.97	0.65
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.60	0.64
1:A:214:LEU:HD11	1:A:236:PRO:HB2	1.79	0.64
1:A:237:GLU:N	1:A:237:GLU:OE1	2.31	0.64
1:A:962:ARG:CG	1:A:962:ARG:HH11	2.11	0.64
1:A:548:ARG:O	1:A:552:VAL:HG13	1.98	0.63
1:A:255:PRO:HD2	1:A:258:HIS:ND1	2.13	0.62
1:A:364:ASN:O	1:A:366:CYS:N	2.32	0.62
1:A:187:ASN:N	1:A:210:LYS:HD3	2.15	0.62
1:A:553:THR:HG22	1:A:564:MET:CE	2.30	0.61
1:A:512:ARG:O	1:A:515:LEU:HG	2.01	0.61
1:A:367:SER:CB	1:A:368:GLU:C	2.65	0.61
1:A:328:ILE:HG22	1:A:329:GLU:HG2	1.82	0.61
1:A:553:THR:CG2	1:A:564:MET:CE	2.78	0.60
1:A:855:LEU:C	1:A:855:LEU:HD23	2.23	0.59
1:A:895:HIS:H	1:A:898:ASN:HD21	1.48	0.59
1:A:318:SER:HB2	1:A:319:LEU:HD23	1.83	0.59
1:A:245:GLY:HA3	1:A:768:ALA:CB	2.26	0.59
1:A:211:ASP:O	1:A:256:LEU:HG	2.03	0.59
1:A:689:LEU:HD21	1:A:824:LEU:HD11	1.84	0.59
1:A:343:VAL:HB	1:A:360:SER:OG	2.02	0.59
1:A:193:ASN:HD21	1:A:202:SER:HB2	1.68	0.59
1:A:355:CYS:HB2	1:A:378:ASP:HB3	1.84	0.58
1:A:549:LEU:HG	1:A:564:MET:HE3	1.85	0.58
1:A:553:THR:CG2	1:A:564:MET:HE2	2.34	0.58
1:A:842:SER:O	1:A:844:MET:HG2	2.03	0.58
1:A:782:ASP:HA	1:A:821:ARG:NH1	2.18	0.58
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.37	0.57
1:A:146:PHE:CE1	1:A:631:LYS:HE2	2.39	0.56
1:A:1012:LEU:O	1:A:1016:ARG:HG3	2.04	0.56
1:A:532:TRP:HZ3	1:A:564:MET:CE	2.18	0.56
1:A:432:LEU:HB3	1:A:483:VAL:HG23	1.88	0.56
1:A:209:THR:HB	1:A:257:CYS:HB3	1.87	0.56
1:A:435:GLY:HA2	1:A:475:LEU:O	2.05	0.56
1:A:367:SER:HB2	1:A:368:GLU:CA	2.35	0.56
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.71	0.55
1:A:364:ASN:C	1:A:366:CYS:H	2.09	0.55
1:A:907:LEU:C	1:A:907:LEU:HD23	2.27	0.55
1:A:439:LEU:O	1:A:470:ALA:HA	2.05	0.55
1:A:205:PHE:CZ	1:A:223:LYS:HG3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:MET:O	1:A:719:MET:HG3	2.06	0.54
1:A:116:GLN:HB3	1:A:683:MET:SD	2.47	0.54
1:A:618:VAL:O	1:A:621:TYR:HB2	2.07	0.54
1:A:383:ASP:HA	1:A:558:HIS:HB3	1.89	0.54
1:A:617:GLN:HE22	1:A:620:LYS:NZ	2.06	0.53
1:A:278:HIS:CD2	1:A:280:SER:H	2.26	0.53
1:A:437:ARG:HD3	1:A:475:LEU:HD12	1.90	0.53
1:A:953:PHE:O	1:A:956:PHE:HB3	2.09	0.53
1:A:656:HIS:O	1:A:658:PRO:HD3	2.09	0.53
1:A:367:SER:CB	1:A:368:GLU:CA	2.87	0.53
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.89	0.53
1:A:828:VAL:O	2:A:1500:DLN:H1	2.09	0.53
1:A:929:ARG:HH22	1:A:1001:SER:HB3	1.74	0.53
1:A:716:HIS:O	1:A:720:ARG:HG3	2.07	0.53
1:A:951:GLU:O	1:A:955:ARG:HG3	2.10	0.52
1:A:335:ALA:C	1:A:365:VAL:HG11	2.30	0.52
1:A:110:LYS:HZ2	1:A:144:ARG:HH12	1.56	0.52
1:A:553:THR:HG21	1:A:564:MET:HG2	1.91	0.52
1:A:417:PRO:HB2	1:A:444:SER:HB3	1.91	0.52
1:A:341:LEU:HG	1:A:365:VAL:HA	1.91	0.52
1:A:435:GLY:O	1:A:475:LEU:N	2.40	0.52
1:A:434:THR:HG21	1:A:477:GLU:HA	1.92	0.51
1:A:489:GLU:O	1:A:493:GLU:OE1	2.28	0.51
1:A:620:LYS:HE2	1:A:660:VAL:HG11	1.92	0.51
1:A:324:SER:HA	1:A:375:LEU:O	2.10	0.51
1:A:898:ASN:C	1:A:898:ASN:HD22	2.14	0.51
1:A:330:GLY:O	1:A:368:GLU:HA	2.11	0.51
1:A:432:LEU:HG	1:A:433:LYS:N	2.26	0.51
1:A:346:GLY:HA3	1:A:357:THR:HG22	1.93	0.51
1:A:221:LEU:HD23	1:A:224:LYS:HE2	1.93	0.51
1:A:135:GLU:HG3	1:A:428:TYR:CG	2.47	0.50
1:A:516:GLU:C	1:A:517:ARG:HE	2.15	0.50
1:A:316:LEU:CD1	1:A:318:SER:OG	2.60	0.50
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.47	0.50
1:A:332:LYS:HB3	1:A:469:ALA:HB2	1.94	0.49
1:A:365:VAL:HG13	1:A:365:VAL:O	2.12	0.49
1:A:134:PRO:HA	1:A:137:ASN:HB2	1.94	0.49
1:A:855:LEU:HD22	1:A:941:VAL:HG21	1.95	0.49
1:A:319:LEU:O	1:A:382:CYS:HB3	2.13	0.48
1:A:247:HIS:HB2	1:A:738:SER:HA	1.94	0.48
1:A:367:SER:CB	1:A:368:GLU:HB3	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:THR:HG21	1:A:564:MET:CE	2.44	0.48
1:A:395:TYR:HB3	1:A:417:PRO:HA	1.95	0.48
1:A:779:LYS:CE	1:A:782:ASP:OD2	2.62	0.48
2:A:1500:DLN:CAM	2:A:1500:DLN:H102	2.26	0.48
1:A:432:LEU:HG	1:A:433:LYS:H	1.79	0.47
1:A:589:ASP:OD2	1:A:591:TYR:HB2	2.14	0.47
1:A:553:THR:CG2	1:A:564:MET:HE3	2.43	0.47
1:A:1007:THR:OG1	1:A:1010:GLU:HG3	2.15	0.47
1:A:439:LEU:N	1:A:471:LEU:O	2.46	0.47
1:A:955:ARG:HE	1:A:955:ARG:HB3	1.38	0.47
1:A:221:LEU:CD2	1:A:224:LYS:HE2	2.44	0.47
1:A:918:ASN:HB2	1:A:988:GLU:OE1	2.15	0.47
1:A:759:LEU:O	1:A:777:ILE:HA	2.14	0.47
1:A:488:LEU:HD12	1:A:491:ILE:HB	1.97	0.46
1:A:918:ASN:HB2	1:A:988:GLU:CG	2.45	0.46
1:A:192:VAL:HG11	1:A:216:LEU:HD21	1.97	0.46
1:A:892:GLY:O	1:A:893:ASP:HB3	2.15	0.46
1:A:383:ASP:OD2	1:A:558:HIS:ND1	2.45	0.46
1:A:431:GLN:HB2	1:A:484:TYR:CE1	2.51	0.46
1:A:368:GLU:O	1:A:368:GLU:HG3	2.15	0.46
1:A:325:ILE:CD1	1:A:375:LEU:HD12	2.46	0.46
1:A:895:HIS:O	1:A:898:ASN:ND2	2.49	0.46
1:A:489:GLU:HG3	1:A:490:LYS:N	2.31	0.45
1:A:713:GLU:OE1	1:A:713:GLU:HA	2.16	0.45
1:A:427:ASP:OD1	1:A:431:GLN:N	2.46	0.45
1:A:282:ILE:HA	1:A:285:MET:CE	2.45	0.45
1:A:1008:GLU:O	1:A:1008:GLU:HG2	2.17	0.45
1:A:550:LEU:O	1:A:553:THR:HG23	2.17	0.45
1:A:316:LEU:HD11	1:A:318:SER:OG	2.17	0.45
1:A:720:ARG:HH22	1:A:747:GLU:HG2	1.82	0.45
1:A:553:THR:HG21	1:A:564:MET:HE2	1.98	0.44
1:A:350:GLY:HA2	1:A:585:PHE:CZ	2.53	0.44
1:A:829:LEU:O	1:A:830:HIS:HB2	2.17	0.44
1:A:657:VAL:HB	1:A:660:VAL:HG22	2.00	0.44
1:A:328:ILE:O	1:A:371:TRP:N	2.45	0.44
1:A:434:THR:C	1:A:437:ARG:HH12	2.21	0.44
1:A:955:ARG:NH2	1:A:959:TYR:OH	2.50	0.44
1:A:255:PRO:HD2	1:A:258:HIS:CE1	2.54	0.43
1:A:565:LEU:O	1:A:568:LEU:N	2.51	0.43
1:A:807:ASP:C	1:A:807:ASP:OD1	2.57	0.43
1:A:282:ILE:O	1:A:285:MET:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:ILE:CD1	1:A:901:ILE:CD1	2.97	0.43
1:A:700:LYS:HZ3	1:A:780:ASN:HD22	1.66	0.43
1:A:855:LEU:C	1:A:855:LEU:CD2	2.87	0.42
1:A:205:PHE:HZ	1:A:223:LYS:CB	2.30	0.42
1:A:193:ASN:HD21	1:A:202:SER:CB	2.33	0.42
1:A:282:ILE:HA	1:A:285:MET:HE3	2.02	0.42
1:A:323:PHE:O	1:A:377:PHE:N	2.39	0.42
1:A:381:VAL:C	1:A:383:ASP:H	2.22	0.42
1:A:900:MET:HE1	2:A:1500:DLN:H213	2.01	0.42
1:A:808:LEU:O	1:A:878:SER:HA	2.20	0.42
1:A:374:ARG:CG	1:A:374:ARG:HH11	2.32	0.42
1:A:1023:LEU:HA	1:A:1023:LEU:HD12	1.75	0.42
1:A:907:LEU:HD23	1:A:908:PHE:N	2.35	0.41
1:A:440:TYR:CD1	1:A:470:ALA:HB2	2.55	0.41
1:A:225:ALA:O	1:A:230:GLN:N	2.53	0.41
1:A:437:ARG:O	1:A:472:VAL:HA	2.21	0.41
1:A:434:THR:HA	1:A:475:LEU:HB2	2.03	0.41
1:A:825:ILE:HD13	2:A:1500:DLN:C13	2.50	0.41
1:A:693:LYS:NZ	1:A:697:ASP:OD2	2.53	0.41
1:A:380:SER:O	1:A:383:ASP:HB2	2.20	0.41
1:A:604:THR:OG1	1:A:607:GLU:HG3	2.21	0.41
1:A:349:HIS:HB2	1:A:354:LEU:HD11	2.02	0.41
1:A:332:LYS:HB2	1:A:333:VAL:H	1.75	0.41
1:A:700:LYS:O	1:A:704:GLN:HG3	2.20	0.41
1:A:242:GLN:O	1:A:274:LEU:HA	2.21	0.41
1:A:255:PRO:O	1:A:256:LEU:C	2.59	0.40
1:A:900:MET:CE	2:A:1500:DLN:H213	2.51	0.40
1:A:809:ARG:HH11	1:A:809:ARG:HD2	1.74	0.40
1:A:971:GLY:HA2	1:A:1002:LEU:HD13	2.03	0.40
1:A:316:LEU:HD12	1:A:318:SER:H	1.86	0.40
1:A:146:PHE:HA	1:A:149:GLU:HG3	2.04	0.40
1:A:564:MET:HE2	1:A:564:MET:HB2	1.96	0.40
1:A:614:GLN:HG3	1:A:981:MET:HG2	2.04	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%)	743 (93%)	46 (6%)	11 (1%)	14	28

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	VAL
1	A	366	CYS
1	A	367	SER
1	A	866	GLU
1	A	368	GLU
1	A	478	VAL
1	A	586	SER
1	A	742	GLU
1	A	845	ALA
1	A	911	ASP
1	A	382	CYS

### 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	728/827 (88%)	658 (90%)	70 (10%)	10	20

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	112	LEU
1	A	129	ASP
1	A	130	SER
1	A	132	ARG
1	A	149	GLU
1	A	156	GLN
1	A	166	SER
1	A	187	ASN
1	A	188	ARG
1	A	190	LEU
1	A	192	VAL
1	A	197	GLU
1	A	216	LEU
1	A	219	CYS
1	A	228	PHE
1	A	264	SER
1	A	268	SER
1	A	271	THR
1	A	287	ASP
1	A	316	LEU
1	A	317	TRP
1	A	319	LEU
1	A	331	ARG
1	A	332	LYS
1	A	340	LYS
1	A	342	VAL
1	A	352	GLU
1	A	365	VAL
1	A	366	CYS
1	A	367	SER
1	A	374	ARG
1	A	390	LEU
1	A	397	VAL
1	A	418	ILE
1	A	423	LEU
1	A	434	THR
1	A	472	VAL
1	A	492	LEU
1	A	511	LEU
1	A	512	ARG
1	A	517	ARG
1	A	523	LEU

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Mol	Chain	Res	Type
1	A	525	GLU
1	A	553	THR
1	A	565	LEU
1	A	576	VAL
1	A	684	LYS
1	A	705	LYS
1	A	710	GLN
1	A	731	LEU
1	A	743	GLU
1	A	744	VAL
1	A	752	MET
1	A	754	SER
1	A	770	SER
1	A	787	ASP
1	A	795	GLN
1	A	841	LYS
1	A	842	SER
1	A	847	THR
1	A	898	ASN
1	A	911	ASP
1	A	915	PHE
1	A	930	VAL
1	A	955	ARG
1	A	962	ARG
1	A	990	SER
1	A	1004	LEU
1	A	1024	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	193	ASN
1	A	206	GLN
1	A	278	HIS
1	A	617	GLN
1	A	721	GLN
1	A	780	ASN
1	A	898	ASN
1	A	914	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	DLN	A	1500	-	21,24,24	2.58	3 (14%)	22,34,34	2.82	4 (18%)

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	DLN	A	1500	-	-	0/4/9/9	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	DLN	N8-N7	-10.68	1.24	1.37
2	A	1500	DLN	CAI-CAM	-2.17	1.40	1.43
2	A	1500	DLN	C1-N2	2.46	1.36	1.32



All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	DLN	N2-C1-N6	-8.72	122.22	128.89
2	A	1500	DLN	C4-C5-N10	-2.69	117.42	122.73
2	A	1500	DLN	C15-C16-C17	-2.37	116.86	120.24
2	A	1500	DLN	CAI-N8-N7	8.05	109.99	104.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	DLN	5	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%)	-0.10	19 (2%) 64 57	5, 20, 35, 52	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	LEU	5.6
1	A	366	CYS	5.5
1	A	396	ALA	3.9
1	A	334	ASN	3.8
1	A	342	VAL	3.3
1	A	444	SER	3.0
1	A	397	VAL	2.9
1	A	515	LEU	2.9
1	A	329	GLU	2.9
1	A	330	GLY	2.7
1	A	512	ARG	2.6
1	A	317	TRP	2.5
1	A	483	VAL	2.4
1	A	365	VAL	2.4
1	A	205	PHE	2.3
1	A	340	LYS	2.3
1	A	524	TYR	2.2
1	A	319	LEU	2.2
1	A	370	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 [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	DLN	A	1500	22/22	0.97	0.13	-0.65	18,24,32,40	0

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

There are no such residues in this entry.