



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:23 AM GMT

PDB ID : 2WXR
Title : THE CRYSTAL STRUCTURE OF THE MURINE CLASS IA PI 3-KINASE P110DELTA.
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 : 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

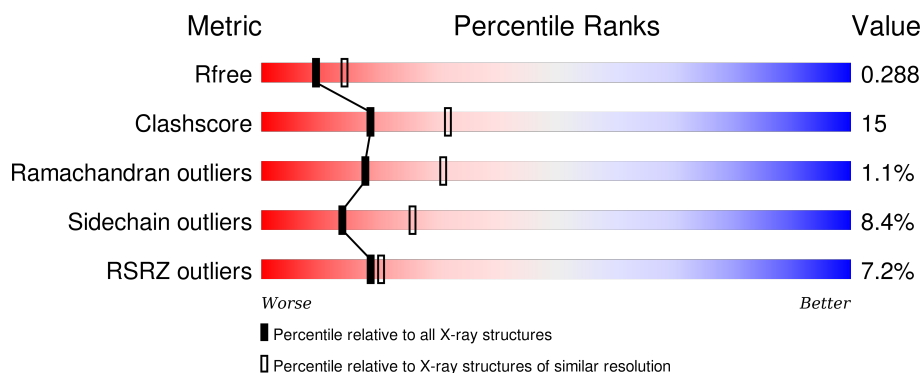
1 Overall quality at a glance

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 ≥ 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>6%</div> <div>57%</div> <div>27%</div> <div>•</div> <div>13%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6702 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

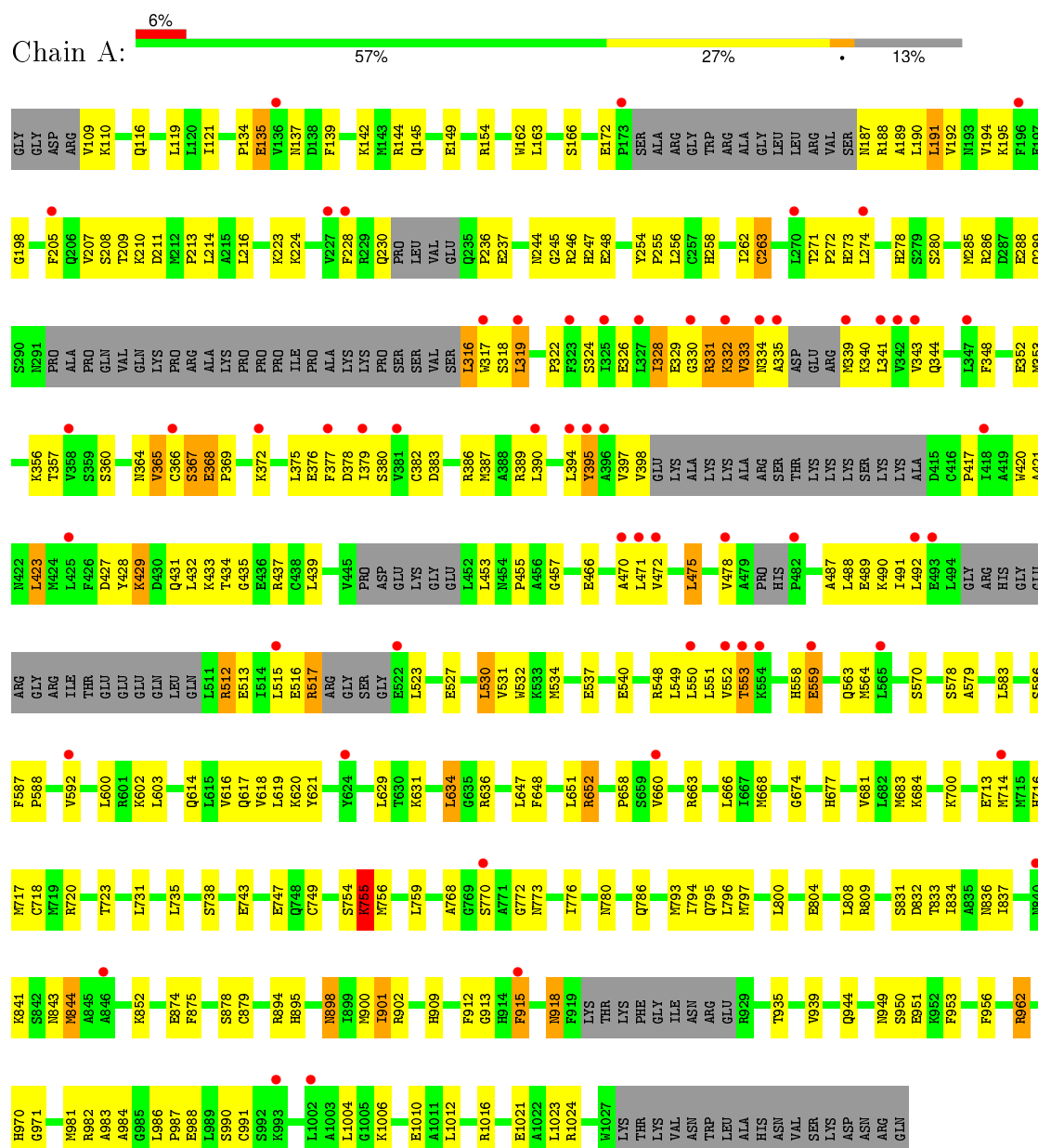
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	69	Total	O	0	0
			69	69		

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, α , β , γ	143.31Å 64.50Å 117.13Å 90.00° 103.94° 90.00°	Depositor
Resolution (Å)	66.96 – 2.50 66.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (66.96-2.50) 95.7 (66.94-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.221 , 0.279 0.230 , 0.288	Depositor DCC
R_{free} test set	1077 reflections (3.21%)	DCC
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 34679 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6702	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0.74	3/6776 (0.0%)	0.78	6/9142 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	326	GLU	CD-OE2	8.95	1.35	1.25
1	A	718	CYS	CB-SG	-6.91	1.70	1.82
1	A	398	VAL	C-O	5.32	1.33	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	902	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	634	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	423	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	652	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	530	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	390	LEU	CA-CB-CG	5.06	126.93	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	205	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	69	0	0	5	0
All	All	6702	0	6615	205	4

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 15.

All (205) 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	1.57	1.25
1:A:841:LYS:HB2	1:A:844:MET:HE1	1.38	1.05
1:A:962:ARG:HG2	1:A:962:ARG:HH11	1.22	1.01
1:A:367:SER:HB3	1:A:369:PRO:N	1.76	0.99
1:A:435:GLY:HA2	1:A:475:LEU:O	1.75	0.85
1:A:549:LEU:HG	1:A:564:MET:CE	2.06	0.85
1:A:944:GLN:HE21	1:A:949:ASN:HD21	1.22	0.83
1:A:549:LEU:HG	1:A:564:MET:HE3	1.58	0.83
1:A:837:ILE:HD13	1:A:901:ILE:HD11	1.60	0.81
1:A:895:HIS:H	1:A:898:ASN:HD21	1.26	0.80
1:A:191:LEU:O	1:A:272:PRO:HD2	1.82	0.79
1:A:331:ARG:HA	1:A:368:GLU:HA	1.62	0.79
1:A:837:ILE:CD1	1:A:901:ILE:HD11	2.12	0.78
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.65	0.78
1:A:982:ARG:NH2	1:A:991:CYS:HA	2.00	0.77
1:A:786:GLN:HG2	1:A:913:GLY:HA2	1.68	0.75
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.69	0.72
1:A:962:ARG:HG2	1:A:962:ARG:NH1	1.96	0.72
1:A:386:ARG:HG3	1:A:387:MET:CE	2.19	0.72
1:A:832:ASP:HB3	1:A:837:ILE:HD11	1.70	0.71
1:A:334:ASN:CG	1:A:335:ALA:H	1.93	0.70
1:A:367:SER:HB3	1:A:368:GLU:CA	2.21	0.69
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.28	0.69
1:A:944:GLN:HE21	1:A:949:ASN:ND2	1.89	0.69
1:A:652:ARG:HD3	1:A:668:MET:HE1	1.74	0.68
1:A:367:SER:CB	1:A:369:PRO:N	2.56	0.68
1:A:843:ASN:O	1:A:844:MET:HG3	1.94	0.68
1:A:648:PHE:CE1	1:A:668:MET:CE	2.77	0.67
1:A:110:LYS:HZ3	1:A:144:ARG:HH12	1.43	0.67
1:A:188:ARG:HD2	1:A:189:ALA:O	1.96	0.66
1:A:549:LEU:O	1:A:553:THR:HG22	1.96	0.66
1:A:335:ALA:C	1:A:365:VAL:HG21	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:PHE:HE2	1:A:453:LEU:HD23	1.61	0.66
1:A:271:THR:O	1:A:273:HIS:HD2	1.79	0.65
1:A:334:ASN:CG	1:A:335:ALA:N	2.48	0.65
1:A:437:ARG:O	1:A:472:VAL:HA	1.96	0.65
1:A:341:LEU:CD1	1:A:365:VAL:HA	2.28	0.64
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.79	0.64
1:A:984:ALA:CB	1:A:986:LEU:HD13	2.27	0.63
1:A:329:GLU:HB2	1:A:369:PRO:O	1.98	0.63
1:A:366:CYS:O	1:A:367:SER:HB2	1.98	0.63
1:A:553:THR:HG21	1:A:564:MET:HE2	1.81	0.62
1:A:895:HIS:H	1:A:898:ASN:ND2	1.96	0.62
1:A:513:GLU:O	1:A:517:ARG:NH2	2.31	0.62
1:A:648:PHE:CE1	1:A:668:MET:HE3	2.35	0.61
1:A:190:LEU:HD22	1:A:209:THR:HG22	1.82	0.61
1:A:614:GLN:HG3	1:A:981:MET:HG2	1.81	0.61
1:A:553:THR:CG2	1:A:564:MET:HE2	2.31	0.61
1:A:935:THR:O	1:A:939:VAL:HG23	2.01	0.61
1:A:116:GLN:HB3	1:A:683:MET:SD	2.40	0.61
1:A:324:SER:HB2	1:A:375:LEU:O	2.01	0.60
1:A:793:MET:O	1:A:797:MET:HG3	2.01	0.60
1:A:192:VAL:HG13	1:A:272:PRO:HB2	1.83	0.60
1:A:549:LEU:HG	1:A:564:MET:HE1	1.83	0.60
1:A:110:LYS:NZ	1:A:144:ARG:HH12	1.99	0.59
1:A:341:LEU:HD12	1:A:365:VAL:HA	1.85	0.59
1:A:339:MET:O	1:A:365:VAL:HG23	2.02	0.59
1:A:832:ASP:HB3	1:A:837:ILE:CD1	2.33	0.59
1:A:435:GLY:O	1:A:475:LEU:N	2.36	0.58
1:A:984:ALA:HB3	1:A:986:LEU:HD13	1.86	0.58
1:A:1021:GLU:O	1:A:1024:ARG:HG2	2.03	0.58
1:A:328:ILE:HG22	1:A:329:GLU:HG2	1.84	0.58
1:A:344:GLN:HB2	1:A:395:TYR:OH	2.03	0.58
1:A:433:LYS:CB	1:A:475:LEU:HD23	2.34	0.57
1:A:553:THR:HG21	1:A:564:MET:HG2	1.85	0.57
1:A:488:LEU:HD12	1:A:491:ILE:HB	1.86	0.57
1:A:365:VAL:HG12	1:A:365:VAL:O	2.04	0.57
1:A:324:SER:HA	1:A:377:PHE:HD2	1.70	0.56
1:A:648:PHE:CE1	1:A:668:MET:HE2	2.39	0.56
1:A:368:GLU:O	1:A:368:GLU:HG3	2.05	0.56
1:A:420:TRP:CH2	1:A:457:GLY:HA3	2.41	0.55
1:A:334:ASN:ND2	1:A:335:ALA:H	2.04	0.54
1:A:383:ASP:HA	1:A:558:HIS:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:LEU:N	1:A:471:LEU:O	2.40	0.54
1:A:618:VAL:HG12	1:A:629:LEU:CD2	2.38	0.54
1:A:278:HIS:HD2	1:A:280:SER:OG	1.91	0.53
1:A:768:ALA:HB3	1:A:772:GLY:HA3	1.91	0.53
1:A:700:LYS:HE3	1:A:756:MET:O	2.09	0.53
1:A:1006:LYS:HD3	1:A:1010:GLU:HB3	1.90	0.53
1:A:549:LEU:CG	1:A:564:MET:HE1	2.38	0.53
1:A:558:HIS:CD2	1:A:559:GLU:N	2.77	0.53
1:A:395:TYR:HB3	1:A:417:PRO:HA	1.90	0.53
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.90	0.53
1:A:343:VAL:H	1:A:360:SER:HB2	1.74	0.52
1:A:154:ARG:HH11	1:A:154:ARG:HG2	1.74	0.52
1:A:984:ALA:HB1	1:A:986:LEU:HD13	1.92	0.52
1:A:553:THR:HG21	1:A:564:MET:CE	2.39	0.52
1:A:588:PRO:HD2	2:A:2009:HOH:O	2.08	0.52
1:A:365:VAL:CG1	1:A:365:VAL:O	2.58	0.52
1:A:617:GLN:NE2	1:A:984:ALA:HA	2.24	0.51
1:A:550:LEU:HA	1:A:553:THR:CG2	2.40	0.51
1:A:335:ALA:N	1:A:365:VAL:HG11	2.25	0.51
1:A:380:SER:O	1:A:383:ASP:HB2	2.09	0.51
1:A:953:PHE:O	1:A:956:PHE:HB3	2.10	0.51
1:A:713:GLU:O	1:A:717:MET:HG3	2.11	0.51
1:A:190:LEU:HD22	1:A:209:THR:CG2	2.41	0.51
1:A:213:PRO:HD3	1:A:254:TYR:O	2.11	0.50
1:A:512:ARG:C	1:A:512:ARG:HE	2.14	0.50
1:A:549:LEU:HA	1:A:552:VAL:HG22	1.93	0.50
1:A:244:ASN:ND2	1:A:273:HIS:HB3	2.26	0.50
1:A:247:HIS:HB2	1:A:738:SER:HA	1.93	0.50
1:A:432:LEU:HG	1:A:433:LYS:N	2.27	0.50
1:A:433:LYS:HB3	1:A:475:LEU:HD23	1.94	0.50
1:A:386:ARG:HG3	1:A:387:MET:HE3	1.93	0.49
1:A:537:GLU:HA	1:A:540:GLU:HB2	1.93	0.49
1:A:620:LYS:HE2	1:A:660:VAL:HG11	1.93	0.49
1:A:256:LEU:O	1:A:262:ILE:HB	2.12	0.49
1:A:135:GLU:HG3	1:A:428:TYR:CG	2.47	0.49
1:A:135:GLU:HG3	1:A:428:TYR:CD1	2.47	0.49
1:A:433:LYS:HB2	1:A:475:LEU:HD23	1.94	0.49
1:A:437:ARG:HD3	1:A:475:LEU:HD22	1.94	0.49
1:A:319:LEU:O	1:A:382:CYS:HB3	2.12	0.49
1:A:617:GLN:HE22	1:A:620:LYS:NZ	2.11	0.49
1:A:833:THR:N	1:A:900:MET:HE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1012:LEU:O	1:A:1016:ARG:HG3	2.12	0.49
1:A:187:ASN:N	1:A:210:LYS:HZ2	2.12	0.48
1:A:875:PHE:O	1:A:879:CYS:HB2	2.13	0.48
1:A:145:GLN:O	1:A:149:GLU:HG3	2.12	0.48
1:A:832:ASP:C	1:A:900:MET:HE2	2.34	0.48
1:A:285:MET:O	1:A:288:GLU:HG2	2.13	0.48
1:A:237:GLU:N	1:A:237:GLU:OE1	2.40	0.47
1:A:121:ILE:HA	1:A:668:MET:HE1	1.95	0.47
1:A:353:MET:SD	1:A:357:THR:HG23	2.55	0.47
1:A:636:ARG:HD3	2:A:2022:HOH:O	2.14	0.47
1:A:205:PHE:CZ	1:A:223:LYS:HG3	2.49	0.47
1:A:723:THR:HG23	2:A:2032:HOH:O	2.15	0.47
1:A:332:LYS:HB2	1:A:332:LYS:NZ	2.30	0.47
1:A:154:ARG:NH2	1:A:674:GLY:O	2.48	0.47
1:A:549:LEU:HD11	1:A:564:MET:HE1	1.97	0.46
1:A:786:GLN:HB3	2:A:2038:HOH:O	2.14	0.46
1:A:255:PRO:HD2	1:A:258:HIS:CG	2.50	0.46
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.97	0.46
1:A:918:ASN:CB	1:A:988:GLU:HG2	2.45	0.46
1:A:364:ASN:C	1:A:366:CYS:H	2.19	0.46
1:A:962:ARG:CG	1:A:962:ARG:NH1	2.75	0.46
1:A:700:LYS:CE	1:A:756:MET:O	2.64	0.46
1:A:427:ASP:CG	1:A:429:LYS:H	2.18	0.46
1:A:843:ASN:C	1:A:844:MET:HG3	2.35	0.46
1:A:553:THR:CG2	1:A:564:MET:CE	2.94	0.46
1:A:602:LYS:O	1:A:603:LEU:C	2.54	0.46
1:A:389:ARG:NH1	1:A:455:PRO:O	2.36	0.46
1:A:121:ILE:HG22	1:A:668:MET:HB3	1.98	0.46
1:A:549:LEU:O	1:A:552:VAL:HG22	2.16	0.45
1:A:278:HIS:CD2	1:A:280:SER:H	2.34	0.45
1:A:527:GLU:O	1:A:531:VAL:HG23	2.17	0.45
1:A:834:ILE:HD13	1:A:834:ILE:N	2.32	0.45
1:A:364:ASN:O	1:A:366:CYS:N	2.50	0.45
1:A:324:SER:HB3	1:A:376:GLU:HA	1.99	0.45
1:A:517:ARG:C	1:A:548:ARG:HH22	2.20	0.45
1:A:420:TRP:CE3	1:A:421:ALA:HA	2.53	0.44
1:A:532:TRP:HZ2	1:A:563:GLN:NE2	2.15	0.44
1:A:330:GLY:C	1:A:369:PRO:HD2	2.38	0.44
1:A:796:LEU:O	1:A:800:LEU:HG	2.18	0.44
1:A:987:PRO:O	1:A:990:SER:OG	2.35	0.44
1:A:348:PHE:CE2	1:A:453:LEU:HD23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:PRO:O	1:A:137:ASN:HB2	2.17	0.44
1:A:316:LEU:HD12	1:A:318:SER:H	1.82	0.44
1:A:720:ARG:HH22	1:A:747:GLU:HG2	1.82	0.44
1:A:551:LEU:HD21	1:A:586:SER:HB3	1.99	0.44
1:A:915:PHE:C	1:A:915:PHE:CD2	2.91	0.43
1:A:794:ILE:O	1:A:797:MET:HB2	2.18	0.43
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.82	0.43
1:A:439:LEU:O	1:A:470:ALA:HA	2.18	0.43
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.51	0.43
1:A:324:SER:HA	1:A:377:PHE:CD2	2.53	0.43
1:A:970:HIS:O	1:A:971:GLY:C	2.56	0.42
1:A:549:LEU:CD1	1:A:564:MET:HE1	2.48	0.42
1:A:587:PHE:HB3	1:A:592:VAL:HG11	2.00	0.42
1:A:895:HIS:O	1:A:898:ASN:ND2	2.51	0.42
1:A:844:MET:HE2	1:A:844:MET:HB2	1.72	0.42
1:A:700:LYS:NZ	1:A:780:ASN:O	2.47	0.42
1:A:616:VAL:O	1:A:619:LEU:HB2	2.19	0.42
1:A:211:ASP:O	1:A:256:LEU:HG	2.20	0.42
1:A:809:ARG:HE	1:A:874:GLU:CD	2.23	0.42
1:A:322:PRO:HA	1:A:379:ILE:O	2.19	0.42
1:A:833:THR:O	1:A:837:ILE:HD12	2.20	0.42
1:A:953:PHE:CZ	1:A:1023:LEU:HD22	2.54	0.42
1:A:894:ARG:HD3	1:A:909:HIS:CE1	2.55	0.42
1:A:754:SER:O	1:A:755:LYS:HB2	2.20	0.41
1:A:332:LYS:CD	1:A:369:PRO:HD3	2.50	0.41
1:A:617:GLN:O	1:A:620:LYS:HB2	2.20	0.41
1:A:289:GLN:HG2	1:A:677:HIS:CD2	2.55	0.41
1:A:194:VAL:HA	1:A:274:LEU:O	2.20	0.41
1:A:429:LYS:C	1:A:431:GLN:H	2.23	0.41
1:A:224:LYS:O	1:A:228:PHE:HB2	2.21	0.41
1:A:735:LEU:HD12	1:A:776:ILE:HG22	2.02	0.41
1:A:367:SER:CB	1:A:369:PRO:CA	2.99	0.41
1:A:579:ALA:HB1	1:A:600:LEU:HG	2.02	0.41
1:A:139:PHE:CE2	1:A:666:LEU:HB3	2.55	0.41
1:A:808:LEU:O	1:A:878:SER:HA	2.20	0.41
1:A:172:GLU:HG3	1:A:263:CYS:SG	2.61	0.41
1:A:256:LEU:HB3	1:A:262:ILE:HG13	2.02	0.41
1:A:716:HIS:HE1	1:A:749:CYS:O	2.04	0.41
1:A:489:GLU:HG3	1:A:490:LYS:H	1.85	0.41
1:A:487:ALA:O	1:A:491:ILE:HG12	2.21	0.41
1:A:770:SER:O	1:A:773:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:PHE:CZ	1:A:668:MET:HE3	2.56	0.40
1:A:162:TRP:CE3	1:A:286:ARG:HG3	2.56	0.40
1:A:208:SER:OG	1:A:210:LYS:NZ	2.50	0.40
1:A:194:VAL:HG12	1:A:195:LYS:N	2.36	0.40
1:A:214:LEU:HD11	1:A:236:PRO:HB2	2.04	0.40
1:A:647:LEU:O	1:A:651:LEU:HG	2.21	0.40
1:A:681:VAL:O	1:A:684:LYS:HB3	2.22	0.40
1:A:516:GLU:C	1:A:517:ARG:HE	2.25	0.40
1:A:663:ARG:NH1	2:A:2028:HOH:O	2.43	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:MET:CE	1:A:714:MET:CE[2_555]	0.92	1.28
1:A:714:MET:SD	1:A:714:MET:CE[2_555]	1.23	0.97
1:A:714:MET:SD	1:A:714:MET:SD[2_555]	2.06	0.14
1:A:714:MET:CG	1:A:714:MET:CE[2_555]	2.17	0.03

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%)	738 (92%)	53 (7%)	9 (1%)	17 31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	VAL
1	A	365	VAL
1	A	372	LYS
1	A	198	GLY

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Mol	Chain	Res	Type
1	A	367	SER
1	A	918	ASN
1	A	755	LYS
1	A	368	GLU
1	A	328	ILE

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%)	667 (92%)	61 (8%)	14	25

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	VAL
1	A	119	LEU
1	A	135	GLU
1	A	142	LYS
1	A	163	LEU
1	A	166	SER
1	A	191	LEU
1	A	207	VAL
1	A	230	GLN
1	A	263	CYS
1	A	316	LEU
1	A	317	TRP
1	A	319	LEU
1	A	331	ARG
1	A	332	LYS
1	A	333	VAL
1	A	340	LYS
1	A	352	GLU
1	A	356	LYS
1	A	378	ASP
1	A	394	LEU

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Mol	Chain	Res	Type
1	A	395	TYR
1	A	397	VAL
1	A	423	LEU
1	A	429	LYS
1	A	434	THR
1	A	466	GLU
1	A	475	LEU
1	A	478	VAL
1	A	492	LEU
1	A	512	ARG
1	A	515	LEU
1	A	517	ARG
1	A	523	LEU
1	A	530	LEU
1	A	534	MET
1	A	553	THR
1	A	559	GLU
1	A	570	SER
1	A	578	SER
1	A	631	LYS
1	A	634	LEU
1	A	658	PRO
1	A	731	LEU
1	A	743	GLU
1	A	755	LYS
1	A	759	LEU
1	A	795	GLN
1	A	804	GLU
1	A	831	SER
1	A	836	ASN
1	A	844	MET
1	A	852	LYS
1	A	898	ASN
1	A	901	ILE
1	A	912	PHE
1	A	915	PHE
1	A	950	SER
1	A	951	GLU
1	A	962	ARG
1	A	1004	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	153	HIS
1	A	156	GLN
1	A	193	ASN
1	A	247	HIS
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	344	GLN
1	A	351	ASN
1	A	563	GLN
1	A	617	GLN
1	A	716	HIS
1	A	780	ASN
1	A	898	ASN
1	A	918	ASN
1	A	944	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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 ²)	Q<0.9
1	A	822/940 (87%)	0.62	59 (7%)	18 20	5, 27, 45, 75	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	LEU	10.4
1	A	317	TRP	7.3
1	A	342	VAL	5.0
1	A	334	ASN	4.8
1	A	319	LEU	4.5
1	A	840	ASN	4.4
1	A	846	ALA	4.2
1	A	377	PHE	4.0
1	A	343	VAL	3.9
1	A	472	VAL	3.8
1	A	323	PHE	3.4
1	A	395	TYR	3.4
1	A	471	LEU	3.3
1	A	196	PHE	3.3
1	A	379	ILE	3.3
1	A	515	LEU	3.2
1	A	330	GLY	3.1
1	A	470	ALA	3.1
1	A	327	LEU	3.0
1	A	624	TYR	2.9
1	A	492	LEU	2.9
1	A	205	PHE	2.7
1	A	425	LEU	2.7
1	A	339	MET	2.6
1	A	358	VAL	2.6
1	A	550	LEU	2.6
1	A	390	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	347	LEU	2.5
1	A	366	CYS	2.5
1	A	227	VAL	2.5
1	A	381	VAL	2.4
1	A	372	LYS	2.4
1	A	270	LEU	2.3
1	A	332	LYS	2.3
1	A	482	PRO	2.2
1	A	396	ALA	2.2
1	A	714	MET	2.2
1	A	660	VAL	2.2
1	A	325	ILE	2.2
1	A	274	LEU	2.2
1	A	136	VAL	2.2
1	A	993	LYS	2.2
1	A	228	PHE	2.2
1	A	335	ALA	2.2
1	A	394	LEU	2.1
1	A	565	LEU	2.1
1	A	173	PRO	2.1
1	A	478	VAL	2.1
1	A	418	ILE	2.1
1	A	493	GLU	2.1
1	A	522	GLU	2.1
1	A	1002	LEU	2.0
1	A	553	THR	2.0
1	A	915	PHE	2.0
1	A	559	GLU	2.0
1	A	592	VAL	2.0
1	A	554	LYS	2.0
1	A	552	VAL	2.0
1	A	770	SER	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.