



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:30 AM GMT

PDB ID : 1E8Y  
Title : STRUCTURE DETERMINANTS OF PHOSPHOINOSITIDE 3-KINASE INHIBITION BY WORTMANNIN, LY294002, QUERCETIN, MYRICETIN AND STAUROSPORINE  
Authors : Walker, E.H.; Pacold, M.E.; Perisic, O.; Stephens, L.; Hawkins, P.T.; Wymann, M.P.; Williams, R.L.  
Deposited on : 2000-10-03  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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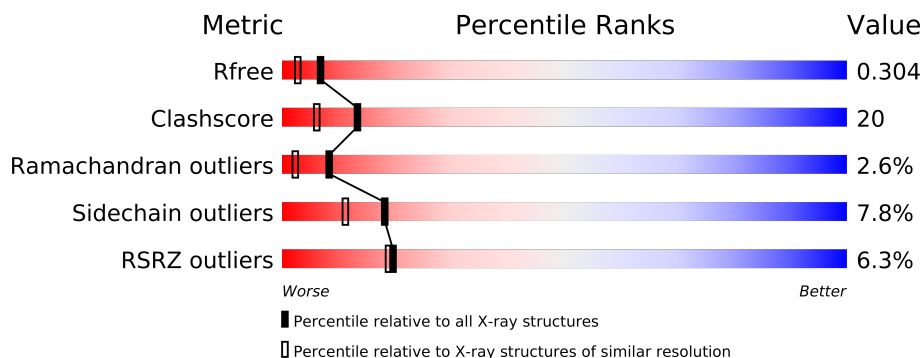
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


The reported resolution of this entry is 2.00 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	966	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6963 atoms, of which 0 are hydrogen and 0 are deuterium.

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 3-KINASE CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6815	4374	1164	1242	35			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	PRO	CLONING ARTEFACT	UNP P48736
A	505	ALA	ARG	CONFLICT	UNP P48736

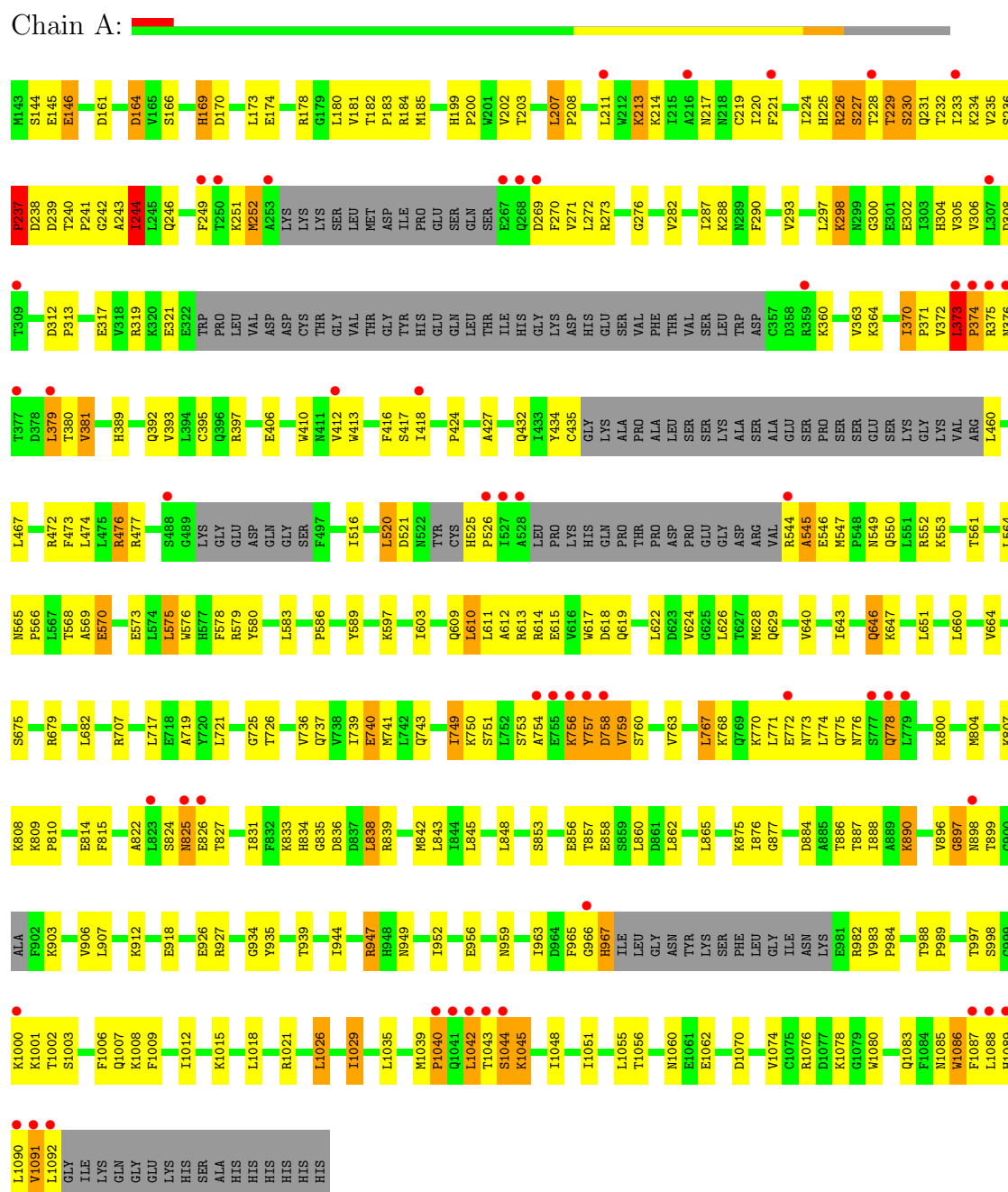
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total	O	0	0
			148	148		

### 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 3-KINASE CATALYTIC SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.23Å 66.25Å 102.64Å 90.00° 97.85° 90.00°	Depositor
Resolution (Å)	68.96 – 2.00 68.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.6 (68.96-2.00) 92.5 (68.96-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.245 , 0.305 0.245 , 0.304	Depositor DCC
$R_{free}$ test set	2284 reflections (3.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 58243 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.73	0/6960	0.78	3/9413 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	947	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	244	ILE	N-CA-C	-5.91	95.03	111.00
1	A	575	LEU	CA-CB-CG	5.61	128.21	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6815	0	6848	278	0
2	A	148	0	0	6	0
All	All	6963	0	6848	278	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (278) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.33	1.11
1:A:525:HIS:HB3	1:A:526:PRO:HD3	1.46	0.94
1:A:373:LEU:HD22	1:A:406:GLU:HG2	1.50	0.93
1:A:804:MET:HE1	1:A:831:ILE:HG12	1.50	0.92
1:A:544:ARG:HH21	1:A:546:GLU:HB3	1.32	0.92
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.21	0.88
1:A:1044:SER:O	1:A:1045:LYS:HG3	1.74	0.86
1:A:576:TRP:CZ3	1:A:579:ARG:HD2	2.12	0.85
1:A:240:THR:O	1:A:244:ILE:HG23	1.78	0.82
1:A:224:ILE:HD13	1:A:233:ILE:HD13	1.64	0.80
1:A:360:LYS:HE2	1:A:417:SER:HA	1.65	0.78
1:A:237:PRO:HA	1:A:287:ILE:HD11	1.65	0.78
1:A:576:TRP:CH2	1:A:579:ARG:HD2	2.18	0.78
1:A:243:ALA:HA	1:A:246:GLN:HG3	1.65	0.77
1:A:379:LEU:HD13	1:A:380:THR:H	1.50	0.75
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.34	0.75
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	1.70	0.74
1:A:217:ASN:HD22	1:A:219:CYS:HB2	1.51	0.74
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.71	0.73
1:A:568:THR:HG22	1:A:570:GLU:H	1.52	0.73
1:A:370:ILE:HD13	1:A:371:PRO:HD2	1.69	0.73
1:A:217:ASN:ND2	1:A:219:CYS:HB2	2.05	0.72
1:A:580:TYR:HE2	1:A:613:ARG:HD3	1.56	0.70
1:A:220:ILE:HD11	1:A:237:PRO:HG3	1.74	0.69
1:A:807:LYS:HD2	1:A:807:LYS:H	1.57	0.69
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.55	0.69
1:A:202:VAL:HG12	1:A:203:THR:N	2.07	0.69
1:A:293:VAL:O	1:A:297:LEU:HG	1.93	0.69
1:A:939:THR:HG21	2:A:2128:HOH:O	1.93	0.68
1:A:1021:ARG:HE	1:A:1056:THR:CG2	2.07	0.68
1:A:888:ILE:HG22	1:A:949:ASN:OD1	1.92	0.68
1:A:1000:LYS:HA	1:A:1076:ARG:NH1	2.08	0.68
1:A:887:THR:HG22	1:A:890:LYS:H	1.58	0.68
1:A:997:THR:HG22	1:A:998:SER:N	2.09	0.68
1:A:174:GLU:HB3	1:A:178:ARG:HH12	1.59	0.68
1:A:1026:LEU:O	1:A:1029:ILE:HG22	1.93	0.67
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.58	0.67
1:A:1043:THR:C	1:A:1045:LYS:H	1.98	0.66
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.77	0.66
1:A:181:VAL:HG12	1:A:185:MET:CE	2.25	0.66
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.26	0.65
1:A:373:LEU:N	1:A:374:PRO:HD2	2.12	0.65
1:A:1060:ASN:HD21	1:A:1062:GLU:HB2	1.60	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:896:VAL:HG12	1:A:897:GLY:H	1.60	0.64
1:A:1002:THR:HG22	1:A:1003:SER:H	1.62	0.64
1:A:804:MET:CE	1:A:810:PRO:HG2	2.28	0.64
1:A:860:LEU:HD11	1:A:1015:LYS:HG2	1.77	0.64
1:A:565:ASN:OD1	1:A:566:PRO:HD2	1.98	0.64
1:A:758:ASP:OD1	1:A:759:VAL:N	2.31	0.64
1:A:170:ASP:OD2	1:A:476:ARG:NH2	2.30	0.63
1:A:886:THR:HG22	1:A:887:THR:H	1.61	0.63
1:A:395:CYS:SG	1:A:418:ILE:HG13	2.39	0.63
1:A:1042:LEU:HD22	1:A:1042:LEU:O	1.99	0.62
1:A:251:LYS:HD3	1:A:251:LYS:O	1.99	0.62
1:A:1006:PHE:O	1:A:1009:PHE:HB3	1.99	0.62
1:A:233:ILE:HD12	1:A:233:ILE:H	1.64	0.62
1:A:1008:LYS:O	1:A:1012:ILE:HG13	1.99	0.62
1:A:231:GLN:HG3	1:A:232:THR:H	1.64	0.62
1:A:379:LEU:HB3	1:A:435:CYS:SG	2.41	0.61
1:A:220:ILE:HD12	1:A:287:ILE:CD1	2.30	0.61
1:A:370:ILE:HD13	1:A:371:PRO:CD	2.30	0.61
1:A:741:MET:HE1	1:A:778:GLN:HB3	1.81	0.61
1:A:888:ILE:HD13	1:A:952:ILE:HG22	1.82	0.61
1:A:982:ARG:HD2	1:A:1090:LEU:HD13	1.83	0.61
1:A:815:PHE:O	1:A:827:THR:HB	2.01	0.61
1:A:888:ILE:CG2	1:A:949:ASN:OD1	2.49	0.60
1:A:768:LYS:O	1:A:772:GLU:HG2	2.01	0.60
1:A:622:LEU:HD21	1:A:651:LEU:HD23	1.82	0.60
1:A:544:ARG:HH21	1:A:546:GLU:CB	2.12	0.60
1:A:568:THR:CG2	1:A:569:ALA:N	2.64	0.60
1:A:886:THR:HG22	1:A:887:THR:N	2.17	0.60
1:A:1043:THR:O	1:A:1045:LYS:N	2.28	0.59
1:A:287:ILE:HD12	1:A:288:LYS:N	2.18	0.59
1:A:614:ARG:HH11	1:A:646:GLN:HE22	1.50	0.59
1:A:221:PHE:HE2	1:A:234:LYS:HD2	1.67	0.59
1:A:568:THR:HG22	1:A:569:ALA:N	2.18	0.59
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.83	0.58
1:A:1060:ASN:ND2	1:A:1062:GLU:H	2.01	0.58
1:A:202:VAL:CG1	1:A:203:THR:N	2.66	0.58
1:A:629:GLN:OE1	2:A:2062:HOH:O	2.17	0.58
1:A:410:TRP:O	1:A:412:VAL:HG23	2.02	0.58
1:A:927:ARG:HE	1:A:959:ASN:HD22	1.50	0.58
1:A:749:ILE:CD1	1:A:770:LYS:HD2	2.33	0.58
1:A:568:THR:HG22	1:A:570:GLU:N	2.19	0.58
1:A:173:LEU:HB2	2:A:2011:HOH:O	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:363:VAL:HG23	1:A:520:LEU:CD1	2.33	0.58
1:A:947:ARG:NH2	1:A:963:ILE:O	2.35	0.58
1:A:757:TYR:HA	1:A:809:LYS:NZ	2.19	0.58
1:A:207:LEU:HD23	1:A:208:PRO:HD2	1.85	0.58
1:A:372:VAL:HG12	1:A:374:PRO:HD2	1.85	0.57
1:A:756:LYS:O	1:A:758:ASP:OD2	2.22	0.57
1:A:379:LEU:HD13	1:A:380:THR:HG22	1.85	0.57
1:A:363:VAL:HG23	1:A:520:LEU:HD13	1.86	0.57
1:A:169:HIS:HE1	2:A:2043:HOH:O	1.87	0.57
1:A:888:ILE:CD1	1:A:952:ILE:HG22	2.34	0.57
1:A:903:LYS:O	1:A:906:VAL:HG23	2.04	0.57
1:A:220:ILE:HD12	1:A:287:ILE:HD11	1.87	0.56
1:A:379:LEU:CD1	1:A:380:THR:H	2.15	0.56
1:A:213:LYS:HD3	1:A:214:LYS:N	2.20	0.56
1:A:614:ARG:HD2	1:A:618:ASP:OD1	2.06	0.56
1:A:774:LEU:O	1:A:776:ASN:N	2.39	0.56
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.36	0.56
1:A:824:SER:OG	1:A:826:GLU:HG3	2.05	0.55
1:A:161:ASP:O	1:A:164:ASP:HB3	2.07	0.55
1:A:615:GLU:O	1:A:619:GLN:HG3	2.07	0.55
1:A:271:VAL:HG23	1:A:282:VAL:HG12	1.89	0.55
1:A:381:VAL:HG22	1:A:434:TYR:O	2.07	0.54
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.89	0.54
1:A:997:THR:HG22	1:A:998:SER:H	1.73	0.54
1:A:1085:ASN:O	1:A:1087:PHE:N	2.41	0.54
1:A:238:ASP:O	1:A:238:ASP:OD1	2.26	0.54
1:A:373:LEU:CD2	1:A:406:GLU:HG2	2.32	0.53
1:A:373:LEU:N	1:A:374:PRO:CD	2.72	0.53
1:A:624:VAL:O	1:A:628:MET:HG2	2.08	0.53
1:A:989:PRO:HG2	1:A:1080:TRP:CD1	2.44	0.53
1:A:180:LEU:C	1:A:183:PRO:HD2	2.29	0.53
1:A:825:ASN:N	1:A:825:ASN:ND2	2.57	0.53
1:A:233:ILE:N	1:A:233:ILE:HD12	2.23	0.52
1:A:804:MET:HE2	1:A:810:PRO:HG2	1.91	0.52
1:A:888:ILE:HD13	1:A:952:ILE:CG2	2.39	0.52
1:A:549:ASN:HD21	1:A:553:LYS:NZ	2.08	0.52
1:A:1042:LEU:O	1:A:1042:LEU:HD13	2.10	0.52
1:A:804:MET:HE3	1:A:810:PRO:HG2	1.91	0.52
1:A:174:GLU:HB3	1:A:178:ARG:NH1	2.24	0.52
1:A:1002:THR:O	1:A:1003:SER:HB3	2.09	0.52
1:A:800:LYS:HD3	1:A:814:GLU:OE1	2.09	0.52
1:A:736:VAL:O	1:A:740:GLU:HB2	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1000:LYS:HA	1:A:1076:ARG:CZ	2.40	0.52
1:A:804:MET:HE1	1:A:831:ILE:CG1	2.33	0.51
1:A:1043:THR:C	1:A:1045:LYS:N	2.62	0.51
1:A:1002:THR:HG22	1:A:1003:SER:N	2.25	0.51
1:A:182:THR:HB	1:A:183:PRO:HD3	1.92	0.51
1:A:611:LEU:O	1:A:614:ARG:HB2	2.10	0.51
1:A:424:PRO:HG2	1:A:427:ALA:HB2	1.92	0.51
1:A:525:HIS:HB3	1:A:526:PRO:CD	2.31	0.51
1:A:1042:LEU:HD22	1:A:1042:LEU:C	2.31	0.51
1:A:569:ALA:O	1:A:573:GLU:HG3	2.11	0.51
1:A:660:LEU:O	1:A:664:VAL:HG23	2.11	0.51
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.26	0.51
1:A:184:ARG:NH2	1:A:321:GLU:OE1	2.43	0.51
1:A:725:GLY:HA3	2:A:2096:HOH:O	2.11	0.50
1:A:317:GLU:O	1:A:726:THR:HG23	2.11	0.50
1:A:839:ARG:HA	1:A:842:MET:HE2	1.93	0.50
1:A:804:MET:HE3	1:A:810:PRO:CG	2.41	0.50
1:A:226:ARG:O	1:A:227:SER:HB2	2.12	0.50
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.93	0.50
1:A:839:ARG:HA	1:A:842:MET:CE	2.42	0.50
1:A:856:GLU:C	1:A:858:GLU:H	2.15	0.50
1:A:235:VAL:HG12	1:A:236:SER:N	2.27	0.50
1:A:373:LEU:H	1:A:374:PRO:CD	2.25	0.49
1:A:544:ARG:O	1:A:545:ALA:HB3	2.12	0.49
1:A:583:LEU:HD23	1:A:583:LEU:O	2.13	0.49
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.32	0.49
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.95	0.49
1:A:860:LEU:HD21	1:A:1015:LYS:CE	2.42	0.49
1:A:750:LYS:NZ	1:A:834:HIS:HD2	2.11	0.49
1:A:308:ASP:N	1:A:308:ASP:OD1	2.45	0.49
1:A:164:ASP:OD1	1:A:166:SER:HB2	2.13	0.49
1:A:774:LEU:C	1:A:776:ASN:N	2.67	0.48
1:A:997:THR:CG2	1:A:998:SER:N	2.76	0.48
1:A:988:THR:HB	1:A:989:PRO:HD2	1.95	0.48
1:A:373:LEU:H	1:A:374:PRO:HD2	1.79	0.48
1:A:242:GLY:O	1:A:246:GLN:HG3	2.13	0.48
1:A:860:LEU:HD21	1:A:1015:LYS:NZ	2.28	0.48
1:A:546:GLU:OE2	1:A:552:ARG:NH1	2.42	0.48
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.95	0.48
1:A:389:HIS:O	1:A:392:GLN:HB3	2.14	0.48
1:A:808:LYS:HD2	1:A:835:GLY:HA3	1.96	0.48
1:A:220:ILE:CD1	1:A:237:PRO:HG3	2.41	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:561:THR:HG21	1:A:565:ASN:ND2	2.28	0.48
1:A:808:LYS:HE3	1:A:836:ASP:OD1	2.14	0.48
1:A:1056:THR:HG23	1:A:1056:THR:O	2.14	0.47
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.78	0.47
1:A:474:LEU:HD23	1:A:525:HIS:N	2.28	0.47
1:A:240:THR:HG22	1:A:242:GLY:H	1.79	0.47
1:A:896:VAL:O	1:A:897:GLY:O	2.32	0.47
1:A:213:LYS:HD3	1:A:214:LYS:H	1.80	0.47
1:A:899:THR:HG22	1:A:899:THR:O	2.15	0.47
1:A:807:LYS:H	1:A:807:LYS:CD	2.26	0.47
1:A:876:ILE:HG12	1:A:877:GLY:N	2.30	0.47
1:A:1042:LEU:CD1	1:A:1042:LEU:H	2.27	0.47
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.49	0.47
1:A:580:TYR:CE2	1:A:613:ARG:HD3	2.44	0.47
1:A:739:ILE:HG13	1:A:740:GLU:N	2.30	0.47
1:A:675:SER:O	1:A:679:ARG:HG3	2.15	0.47
1:A:579:ARG:HG2	1:A:610:LEU:HD11	1.97	0.46
1:A:1055:LEU:O	1:A:1056:THR:HG22	2.15	0.46
1:A:614:ARG:HH11	1:A:646:GLN:NE2	2.11	0.46
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.15	0.46
1:A:544:ARG:NH2	1:A:546:GLU:HB3	2.14	0.46
1:A:935:TYR:O	1:A:939:THR:HG22	2.16	0.46
1:A:213:LYS:NZ	1:A:214:LYS:HB2	2.31	0.46
1:A:825:ASN:HD22	1:A:825:ASN:H	1.64	0.46
1:A:760:SER:O	1:A:763:VAL:HG12	2.15	0.46
1:A:472:ARG:O	1:A:473:PHE:HB2	2.16	0.46
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.97	0.46
1:A:856:GLU:C	1:A:858:GLU:N	2.69	0.46
1:A:1000:LYS:HG2	1:A:1076:ARG:HB3	1.97	0.46
1:A:181:VAL:HG12	1:A:185:MET:HE1	1.95	0.46
1:A:757:TYR:HA	1:A:809:LYS:HZ1	1.81	0.46
1:A:739:ILE:O	1:A:743:GLN:HG3	2.15	0.46
1:A:202:VAL:CG1	1:A:203:THR:H	2.28	0.46
1:A:862:LEU:HB3	1:A:934:GLY:HA3	1.98	0.46
1:A:1042:LEU:HD23	1:A:1048:ILE:HD11	1.98	0.46
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.97	0.45
1:A:233:ILE:CD1	1:A:233:ILE:H	2.29	0.45
1:A:589:TYR:CD1	1:A:589:TYR:N	2.83	0.45
1:A:211:LEU:HD21	1:A:298:LYS:HA	1.97	0.45
1:A:224:ILE:HD12	1:A:224:ILE:N	2.31	0.45
1:A:757:TYR:HD1	1:A:757:TYR:O	1.98	0.45
1:A:467:LEU:O	1:A:476:ARG:HD2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:884:ASP:HB3	1:A:956:GLU:HG3	1.98	0.45
1:A:381:VAL:HA	1:A:434:TYR:O	2.16	0.45
1:A:884:ASP:O	1:A:956:GLU:HG3	2.16	0.45
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.82	0.45
1:A:939:THR:OG1	1:A:944:ILE:HG13	2.17	0.45
1:A:965:PHE:O	1:A:967:HIS:N	2.50	0.45
1:A:181:VAL:CG1	1:A:185:MET:HE1	2.47	0.45
1:A:1018:LEU:HB2	2:A:2141:HOH:O	2.16	0.45
1:A:516:ILE:HG23	1:A:516:ILE:O	2.17	0.45
1:A:622:LEU:CD2	1:A:651:LEU:HD23	2.46	0.44
1:A:737:GLN:O	1:A:741:MET:HG3	2.17	0.44
1:A:237:PRO:HA	1:A:287:ILE:CD1	2.41	0.44
1:A:628:MET:HB2	1:A:1029:ILE:HD12	2.00	0.44
1:A:547:MET:HG2	1:A:578:PHE:CD2	2.52	0.44
1:A:181:VAL:CG1	1:A:185:MET:CE	2.95	0.44
1:A:579:ARG:HG2	1:A:610:LEU:CD1	2.47	0.43
1:A:767:LEU:HD22	1:A:771:LEU:HG	2.00	0.43
1:A:544:ARG:CG	1:A:545:ALA:N	2.82	0.43
1:A:1086:TRP:C	1:A:1087:PHE:CD1	2.92	0.43
1:A:276:GLY:HA3	1:A:822:ALA:HA	1.99	0.43
1:A:912:LYS:HE2	1:A:918:GLU:OE2	2.19	0.43
1:A:287:ILE:HA	1:A:290:PHE:CD1	2.53	0.43
1:A:273:ARG:O	1:A:306:VAL:HG12	2.18	0.43
1:A:640:VAL:O	1:A:643:ILE:HG12	2.18	0.43
1:A:1021:ARG:NE	1:A:1056:THR:CG2	2.78	0.43
1:A:810:PRO:HB3	1:A:833:LYS:HB2	1.99	0.43
1:A:146:GLU:OE2	1:A:319:ARG:NH1	2.51	0.43
1:A:249:PHE:HZ	1:A:270:PHE:HD1	1.67	0.42
1:A:853:SER:O	1:A:857:THR:HG23	2.20	0.42
1:A:875:LYS:HB2	1:A:875:LYS:HE3	1.80	0.42
1:A:229:THR:O	1:A:230:SER:HB3	2.19	0.42
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.01	0.42
1:A:825:ASN:N	1:A:825:ASN:HD22	2.16	0.42
1:A:364:LYS:HB2	1:A:413:TRP:CE3	2.55	0.42
1:A:544:ARG:CG	1:A:545:ALA:H	2.29	0.42
1:A:184:ARG:HD3	1:A:719:ALA:O	2.20	0.42
1:A:241:PRO:HG2	1:A:290:PHE:CZ	2.55	0.42
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.50	0.42
1:A:982:ARG:HD2	1:A:1090:LEU:CD1	2.49	0.42
1:A:239:ASP:HB3	1:A:244:ILE:HG22	2.02	0.42
1:A:1086:TRP:O	1:A:1087:PHE:CD1	2.72	0.42
1:A:860:LEU:HD21	1:A:1015:LYS:HD3	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1086:TRP:HH2	1:A:1090:LEU:HB3	1.85	0.41
1:A:757:TYR:O	1:A:758:ASP:HB3	2.20	0.41
1:A:207:LEU:CD2	1:A:208:PRO:HD2	2.49	0.41
1:A:774:LEU:C	1:A:776:ASN:H	2.23	0.41
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.20	0.41
1:A:199:HIS:O	1:A:200:PRO:C	2.57	0.41
1:A:174:GLU:OE1	1:A:178:ARG:NH1	2.53	0.41
1:A:397:ARG:HA	1:A:397:ARG:HD3	1.86	0.41
1:A:589:TYR:HD1	1:A:589:TYR:N	2.18	0.41
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.51	0.41
1:A:252:MET:HE2	1:A:252:MET:HA	2.02	0.41
1:A:225:HIS:HE1	1:A:304:HIS:CD2	2.23	0.41
1:A:721:LEU:HA	1:A:721:LEU:HD23	1.97	0.41
1:A:609:GLN:O	1:A:612:ALA:HB3	2.20	0.41
1:A:372:VAL:CG1	1:A:374:PRO:HD2	2.51	0.41
1:A:380:THR:O	1:A:435:CYS:HA	2.21	0.41
1:A:312:ASP:HA	1:A:313:PRO:HD2	1.87	0.41
1:A:597:LYS:HB2	1:A:603:ILE:HD13	2.03	0.41
1:A:773:ASN:O	1:A:776:ASN:HB2	2.21	0.40
1:A:583:LEU:HD23	1:A:583:LEU:C	2.40	0.40
1:A:997:THR:CG2	1:A:998:SER:H	2.33	0.40
1:A:927:ARG:NE	1:A:959:ASN:HD22	2.18	0.40
1:A:1001:LYS:HB3	1:A:1002:THR:H	1.68	0.40
1:A:249:PHE:CZ	1:A:270:PHE:HD1	2.39	0.40
1:A:751:SER:C	1:A:753:SER:H	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	823/966 (85%)	745 (90%)	57 (7%)	21 (3%)	<b>8</b> <b>2</b>

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	227	SER
1	A	230	SER
1	A	758	ASP
1	A	775	GLN
1	A	897	GLY
1	A	966	GLY
1	A	1040	PRO
1	A	1044	SER
1	A	1086	TRP
1	A	756	LYS
1	A	1045	LYS
1	A	373	LEU
1	A	545	ALA
1	A	754	ALA
1	A	1088	LEU
1	A	237	PRO
1	A	759	VAL
1	A	1091	VAL
1	A	374	PRO
1	A	244	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	755/864 (87%)	696 (92%)	59 (8%)	18 11

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	145	GLU
1	A	146	GLU
1	A	164	ASP
1	A	169	HIS
1	A	207	LEU
1	A	213	LYS

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Mol	Chain	Res	Type
1	A	226	ARG
1	A	228	THR
1	A	229	THR
1	A	237	PRO
1	A	252	MET
1	A	269	ASP
1	A	298	LYS
1	A	370	ILE
1	A	373	LEU
1	A	375	ARG
1	A	379	LEU
1	A	381	VAL
1	A	393	VAL
1	A	476	ARG
1	A	477	ARG
1	A	520	LEU
1	A	521	ASP
1	A	550	GLN
1	A	570	GLU
1	A	575	LEU
1	A	586	PRO
1	A	610	LEU
1	A	626	LEU
1	A	646	GLN
1	A	647	LYS
1	A	682	LEU
1	A	707	ARG
1	A	717	LEU
1	A	740	GLU
1	A	749	ILE
1	A	757	TYR
1	A	767	LEU
1	A	778	GLN
1	A	825	ASN
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	865	LEU
1	A	890	LYS
1	A	898	ASN
1	A	907	LEU

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Mol	Chain	Res	Type
1	A	926	GLU
1	A	967	HIS
1	A	1026	LEU
1	A	1029	ILE
1	A	1042	LEU
1	A	1051	ILE
1	A	1078	LYS
1	A	1089	HIS
1	A	1091	VAL
1	A	1092	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	153	GLN
1	A	169	HIS
1	A	217	ASN
1	A	225	HIS
1	A	304	HIS
1	A	391	GLN
1	A	483	HIS
1	A	549	ASN
1	A	629	GLN
1	A	646	GLN
1	A	743	GLN
1	A	766	GLN
1	A	773	ASN
1	A	825	ASN
1	A	834	HIS
1	A	908	ASN
1	A	959	ASN
1	A	1005	HIS
1	A	1041	GLN
1	A	1060	ASN
1	A	1083	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	841/966 (87%)	0.34	53 (6%) 19 19	17, 39, 75, 126	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	THR	12.6
1	A	1089	HIS	7.1
1	A	1090	LEU	7.0
1	A	1044	SER	6.7
1	A	253	ALA	6.0
1	A	1092	LEU	5.6
1	A	376	ASN	5.6
1	A	216	ALA	5.4
1	A	249	PHE	4.9
1	A	757	TYR	4.8
1	A	373	LEU	4.5
1	A	823	LEU	4.3
1	A	250	THR	4.1
1	A	1041	GLN	3.7
1	A	755	GLU	3.6
1	A	528	ALA	3.5
1	A	756	LYS	3.5
1	A	1088	LEU	3.4
1	A	1087	PHE	3.4
1	A	777	SER	3.4
1	A	379	LEU	3.2
1	A	269	ASP	3.2
1	A	228	THR	3.2
1	A	1040	PRO	3.1
1	A	1000	LYS	3.0
1	A	544	ARG	2.9
1	A	359	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	779	LEU	2.8
1	A	488	SER	2.7
1	A	375	ARG	2.7
1	A	772	GLU	2.6
1	A	233	ILE	2.6
1	A	412	VAL	2.6
1	A	754	ALA	2.5
1	A	307	LEU	2.4
1	A	778	GLN	2.4
1	A	966	GLY	2.4
1	A	526	PRO	2.4
1	A	374	PRO	2.3
1	A	267	GLU	2.3
1	A	1091	VAL	2.3
1	A	221	PHE	2.2
1	A	309	THR	2.2
1	A	898	ASN	2.2
1	A	418	ILE	2.2
1	A	825	ASN	2.2
1	A	268	GLN	2.2
1	A	211	LEU	2.2
1	A	1042	LEU	2.1
1	A	1043	THR	2.1
1	A	758	ASP	2.1
1	A	527	ILE	2.0
1	A	826	GLU	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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.