



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:55 am BST

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 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

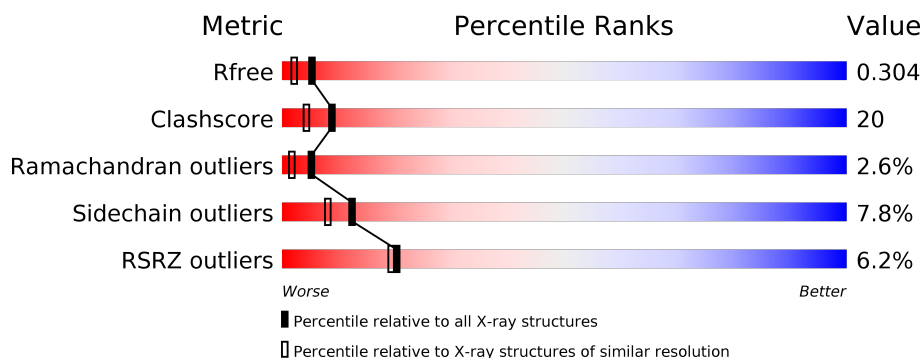
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 respectively. 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	966	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6963 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 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 artifact	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		



L1090		
V1091		
L1092		
GLY		
ILE		
LYS		
GLN		
GLY		
GLU		
LYS		
HIS		
SER		
ALA		
HIS		
HIS		
HIS		
HIS		
HIS		
HIS		

## 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 0.244 , 0.304	Depositor DCC
$R_{free}$ test set	2287 reflections (3.93%)	wwPDB-VP
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 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.73	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( $^{\circ}$ )	Ideal( $^{\circ}$ )
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 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	6815	0	6848	278	0
2	A	148	0	0	6	0
All	All	6963	0	6848	278	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 20.

All (278) 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: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:395:CYS:HB3	1:A:416:PHE:HD2	1.55	0.69
1:A:807:LYS:HD2	1:A:807:LYS:H	1.57	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:174:GLU:HB3	1:A:178:ARG:HH12	1.59	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: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:1060:ASN:HD21	1:A:1062:GLU:HB2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LEU:N	1:A:374:PRO:HD2	2.12	0.65
1:A:1002:THR:HG22	1:A:1003:SER:H	1.62	0.64
1:A:896:VAL:HG12	1:A:897:GLY:H	1.60	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:1006:PHE:O	1:A:1009:PHE:HB3	1.99	0.62
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:1008:LYS:O	1:A:1012:ILE:HG13	1.99	0.62
1:A:233:ILE:HD12	1:A:233:ILE:H	1.64	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: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:HD13	1:A:952:ILE:HG22	1.82	0.61
1:A:768:LYS:O	1:A:772:GLU:HG2	2.01	0.60
1:A:888:ILE:CG2	1:A:949:ASN:OD1	2.49	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:1060:ASN:ND2	1:A:1062:GLU:H	2.01	0.58
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.83	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:749:ILE:CD1	1:A:770:LYS:HD2	2.33	0.58
1:A:927:ARG:HE	1:A:959:ASN:HD22	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:HB2	2:A:2011:HOH:O	2.02	0.58
1:A:363:VAL:HG23	1:A:520:LEU:CD1	2.33	0.58
1:A:568:THR:HG22	1:A:570:GLU:N	2.19	0.58
1:A:947:ARG:NH2	1:A:963:ILE:O	2.35	0.58
1:A:207:LEU:HD23	1:A:208:PRO:HD2	1.85	0.58
1:A:757:TYR:HA	1:A:809:LYS:NZ	2.19	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:169:HIS:HE1	2:A:2043:HOH:O	1.87	0.57
1:A:363:VAL:HG23	1:A:520:LEU:HD13	1.86	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: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:997:THR:HG22	1:A:998:SER:H	1.73	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:549:ASN:HD21	1:A:553:LYS:NZ	2.08	0.52
1:A:888:ILE:HD13	1:A:952:ILE:CG2	2.39	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:1002:THR:O	1:A:1003:SER:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLU:HB3	1:A:178:ARG:NH1	2.24	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
1:A:1000:LYS:HA	1:A:1076:ARG:CZ	2.40	0.52
1:A:1043:THR:C	1:A:1045:LYS:N	2.62	0.51
1:A:804:MET:HE1	1:A:831:ILE:CG1	2.33	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:226:ARG:O	1:A:227:SER:HB2	2.12	0.50
1:A:804:MET:HE3	1:A:810:PRO:CG	2.41	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:O	1:A:583:LEU:HD23	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:750:LYS:NZ	1:A:834:HIS:HD2	2.11	0.49
1:A:860:LEU:HD21	1:A:1015:LYS:CE	2.42	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:988:THR:HB	1:A:989:PRO:HD2	1.95	0.48
1:A:997:THR:CG2	1:A:998:SER:N	2.76	0.48
1:A:373:LEU:H	1:A:374:PRO:HD2	1.79	0.48
1:A:860:LEU:HD21	1:A:1015:LYS:NZ	2.28	0.48
1:A:242:GLY:O	1:A:246:GLN:HG3	2.13	0.48
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:HIS:O	1:A:392:GLN:HB3	2.14	0.48
1:A:546:GLU:OE2	1:A:552:ARG:NH1	2.42	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
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:240:THR:HG22	1:A:242:GLY:H	1.79	0.47
1:A:474:LEU:HD23	1:A:525:HIS:N	2.28	0.47
1:A:213:LYS:HD3	1:A:214:LYS:H	1.80	0.47
1:A:896:VAL:O	1:A:897:GLY:O	2.32	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:1003:SER:O	1:A:1007:GLN:HG3	2.15	0.46
1:A:614:ARG:HH11	1:A:646:GLN:NE2	2.11	0.46
1:A:213:LYS:NZ	1:A:214:LYS:HB2	2.31	0.46
1:A:472:ARG:O	1:A:473:PHE:HB2	2.16	0.46
1:A:544:ARG:NH2	1:A:546:GLU:HB3	2.14	0.46
1:A:760:SER:O	1:A:763:VAL:HG12	2.15	0.46
1:A:825:ASN:HD22	1:A:825:ASN:H	1.64	0.46
1:A:935:TYR:O	1:A:939:THR:HG22	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:739:ILE:O	1:A:743:GLN:HG3	2.15	0.46
1:A:757:TYR:HA	1:A:809:LYS:HZ1	1.81	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:211:LEU:HD21	1:A:298:LYS:HA	1.97	0.45
1:A:233:ILE:CD1	1:A:233:ILE:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.97	0.45
1:A:589:TYR:CD1	1:A:589:TYR:N	2.83	0.45
1:A:224:ILE:HD12	1:A:224:ILE:N	2.31	0.45
1:A:467:LEU:O	1:A:476:ARG:HD2	2.17	0.45
1:A:757:TYR:O	1:A:757:TYR:HD1	1.98	0.45
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:1018:LEU:HB2	2:A:2141:HOH:O	2.16	0.45
1:A:181:VAL:CG1	1:A:185:MET:HE1	2.47	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:628:MET:HB2	1:A:1029:ILE:HD12	2.00	0.44
1:A:237:PRO:HA	1:A:287:ILE:CD1	2.41	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:146:GLU:OE2	1:A:319:ARG:NH1	2.51	0.43
1:A:810:PRO:HB3	1:A:833:LYS:HB2	1.99	0.43
1:A:249:PHE:HZ	1:A:270:PHE:HD1	1.67	0.42
1:A:229:THR:O	1:A:230:SER:HB3	2.19	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:364:LYS:HB2	1:A:413:TRP:CE3	2.55	0.42
1:A:825:ASN:N	1:A:825:ASN:HD22	2.16	0.42
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1086:TRP:O	1:A:1087:PHE:CD1	2.72	0.42
1:A:239:ASP:HB3	1:A:244:ILE:HG22	2.02	0.42
1:A:1086:TRP:HH2	1:A:1090:LEU:HB3	1.85	0.41
1:A:860:LEU:HD21	1:A:1015:LYS:HD3	2.02	0.41
1:A:757:TYR:O	1:A:758:ASP:HB3	2.20	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: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: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:252:MET:HE2	1:A:252:MET:HA	2.02	0.41
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.51	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:312:ASP:HA	1:A:313:PRO:HD2	1.87	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:597:LYS:HB2	1:A:603:ILE:HD13	2.03	0.41
1:A:583:LEU:C	1:A:583:LEU:HD23	2.40	0.40
1:A:773:ASN:O	1:A:776:ASN:HB2	2.21	0.40
1:A:927:ARG:NE	1:A:959:ASN:HD22	2.18	0.40
1:A:997:THR:CG2	1:A:998:SER:H	2.33	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 [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	823/966 (85%)	745 (90%)	57 (7%)	21 (3%)	5 2

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%)	12 8

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
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

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Mol	Chain	Res	Type
1	A	845	LEU
1	A	848	LEU
1	A	865	LEU
1	A	890	LYS
1	A	898	ASN
1	A	907	LEU
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 [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 [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	841/966 (87%)	0.39	52 (6%)	20 19	17, 39, 75, 126	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	THR	12.3
1	A	1090	LEU	8.5
1	A	1044	SER	8.1
1	A	1089	HIS	7.9
1	A	376	ASN	5.7
1	A	1092	LEU	5.7
1	A	757	TYR	5.6
1	A	253	ALA	5.6
1	A	216	ALA	5.4
1	A	250	THR	5.2
1	A	249	PHE	5.2
1	A	373	LEU	5.1
1	A	755	GLU	4.5
1	A	823	LEU	4.0
1	A	756	LYS	3.9
1	A	1000	LYS	3.7
1	A	379	LEU	3.7
1	A	528	ALA	3.7
1	A	777	SER	3.6
1	A	1087	PHE	3.5
1	A	1041	GLN	3.5
1	A	1040	PRO	3.4
1	A	779	LEU	3.4
1	A	269	ASP	3.3
1	A	526	PRO	3.2
1	A	228	THR	3.1
1	A	412	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1088	LEU	3.0
1	A	359	ARG	2.9
1	A	233	ILE	2.9
1	A	488	SER	2.7
1	A	1091	VAL	2.7
1	A	825	ASN	2.6
1	A	966	GLY	2.6
1	A	211	LEU	2.6
1	A	754	ALA	2.5
1	A	374	PRO	2.5
1	A	544	ARG	2.5
1	A	898	ASN	2.4
1	A	772	GLU	2.4
1	A	375	ARG	2.4
1	A	758	ASP	2.4
1	A	164	ASP	2.3
1	A	824	SER	2.3
1	A	309	THR	2.2
1	A	999	GLY	2.2
1	A	418	ILE	2.2
1	A	307	LEU	2.2
1	A	236	SER	2.1
1	A	1042	LEU	2.1
1	A	1043	THR	2.1
1	A	778	GLN	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.