



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 11:38 PM GMT

PDB ID : 1E7U  
Title : STRUCTURE DETERMINANTS OF PHOSPHOINOSITIDE 3-KINASE INHIBITION BY WORTMANNIN, LY294002, QUERCETIN, MYRICETIN AND STAUROSPORINE  
Authors : Walker, E.H.; Perisic, O.; Ried, C.; Stephens, L.; Williams, R.L.  
Deposited on : 2000-09-08  
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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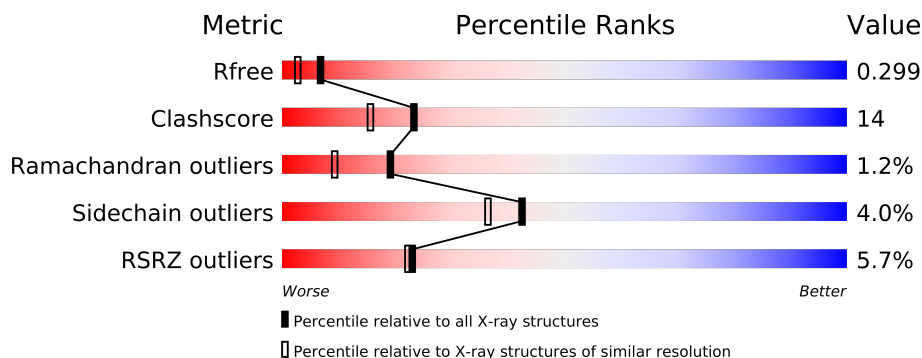
The following versions of software and data (see [references](#)) were used in the production of this report:

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	961	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	KWT	A	1833	-	X

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7249 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.

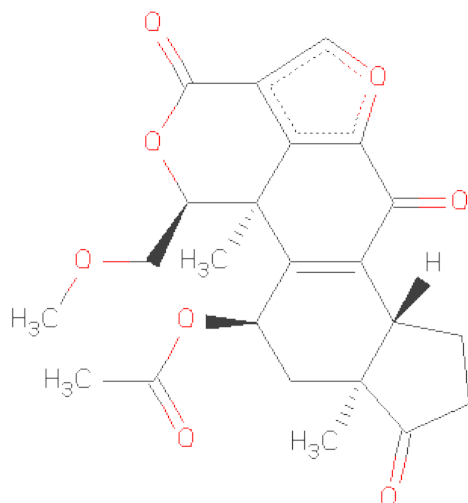
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	872	7054	4530	1205	1282	37	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	ALA	PRO	EXPRESSION TAG	UNP O02697
A	505	ALA	ARG	CONFLICT	UNP O02697

- Molecule 2 is (1S,6BR,9AS,11R,11BR)-9A,11B-DIMETHYL-1-[(METHYLOXY)METHYL]-3,6,9-TRIOXO-1,6,6B,7,8,9,9A,10,11,11B-DECAHYDRO-3H-FURO[4,3,2-DE]INDENO[4,5-H][2]BENZOPYRAN-11-YLACETATE (three-letter code: KWT) (formula: C<sub>23</sub>H<sub>24</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	31	23	8	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	164	Total 164	O 164	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.33Å 67.66Å 106.65Å 90.00° 95.05° 90.00°	Depositor
Resolution (Å)	72.38 – 2.00 72.38 – 1.98	Depositor EDS
% Data completeness (in resolution range)	94.3 (72.38-2.00) 95.7 (72.38-1.98)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 1.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.254 , 0.298 0.253 , 0.299	Depositor DCC
$R_{free}$ test set	2685 reflections (3.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 68702 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% 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

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

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	0.38	0/7202	0.58	0/9742

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	523	TYR	Sidechain

### 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	7054	0	7126	206	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	0	23	0	0
3	A	164	0	0	7	0
All	All	7249	0	7149	206	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 14.

All (206) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:833:LYS:HD3	1:A:838:LEU:HD21	1.38	1.05
1:A:760:SER:HB2	1:A:762:GLN:HE21	1.39	0.88
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.55	0.88
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.23	0.83
1:A:833:LYS:CD	1:A:838:LEU:HD21	2.10	0.80
1:A:497:PHE:HB3	1:A:1042:LEU:HB3	1.62	0.79
1:A:744:LYS:HB2	1:A:744:LYS:NZ	1.99	0.77
1:A:226:ARG:HB3	1:A:229:THR:HB	1.65	0.77
1:A:196:TYR:OH	1:A:728:MET:HE3	1.84	0.77
1:A:772:GLU:HG2	1:A:798:ILE:HD13	1.67	0.76
1:A:351:THR:HG22	1:A:352:VAL:HG23	1.68	0.75
1:A:689:LYS:HG2	1:A:728:MET:CE	2.18	0.73
1:A:207:LEU:HD11	1:A:288:LYS:HD2	1.70	0.72
1:A:425:LYS:HA	1:A:469:ILE:HD12	1.72	0.72
1:A:352:VAL:HG13	1:A:527:ILE:HD12	1.71	0.72
1:A:154:LEU:O	1:A:158:ILE:HG12	1.92	0.70
1:A:576:TRP:O	1:A:579:ARG:HG3	1.91	0.70
1:A:1048:ILE:O	1:A:1051:ILE:HG22	1.94	0.67
1:A:403:PRO:HG2	3:A:2029:HOH:O	1.96	0.65
1:A:949:ASN:N	1:A:1083:GLN:HE22	1.94	0.65
1:A:583:LEU:HD13	1:A:610:LEU:HD22	1.79	0.65
1:A:804:MET:HE1	1:A:812:TRP:HE3	1.61	0.64
1:A:1024:THR:O	1:A:1028:ILE:HG12	1.97	0.64
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.27	0.64
1:A:208:PRO:HD2	1:A:211:LEU:HD12	1.79	0.64
1:A:1010:GLN:O	1:A:1014:VAL:HG23	1.98	0.63
1:A:611:LEU:O	1:A:614:ARG:HG3	1.98	0.63
1:A:807:LYS:HD2	1:A:807:LYS:H	1.63	0.63
1:A:768:LYS:O	1:A:772:GLU:HG3	1.98	0.63
1:A:271:VAL:HB	1:A:310:PRO:HG3	1.80	0.63
1:A:887:THR:HG21	1:A:950:ASP:OD1	1.99	0.62
1:A:567:LEU:HD21	1:A:591:LYS:HD2	1.82	0.62
1:A:689:LYS:HG2	1:A:728:MET:HE1	1.79	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:733:THR:HG22	1:A:737:GLN:HE21	1.65	0.61
1:A:353:SER:HB3	1:A:526:PRO:HA	1.81	0.61
1:A:689:LYS:HG2	1:A:728:MET:HE2	1.83	0.61
1:A:602:GLU:H	1:A:602:GLU:CD	2.04	0.60
1:A:640:VAL:O	1:A:643:ILE:HG12	2.01	0.60
1:A:844:ILE:O	1:A:848:LEU:HD13	2.00	0.60
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	2.17	0.60
1:A:158:ILE:HD11	1:A:721:LEU:HD12	1.84	0.60
1:A:591:LYS:HG2	3:A:2055:HOH:O	2.02	0.60
1:A:235:VAL:HG11	1:A:244:ILE:CD1	2.32	0.60
1:A:354:LEU:HB3	1:A:529:LEU:HD11	1.84	0.59
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.85	0.58
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.34	0.58
1:A:601:GLN:HG3	1:A:602:GLU:N	2.17	0.57
1:A:947:ARG:HH21	1:A:962:HIS:HB3	1.69	0.57
1:A:196:TYR:OH	1:A:728:MET:CE	2.52	0.57
1:A:887:THR:HG22	1:A:889:ALA:H	1.68	0.57
1:A:689:LYS:HE2	1:A:728:MET:HE2	1.85	0.57
1:A:755:GLU:HG2	1:A:807:LYS:O	2.04	0.57
1:A:687:ARG:HH11	1:A:687:ARG:HG3	1.70	0.57
1:A:235:VAL:HG12	1:A:239:ASP:OD2	2.05	0.57
1:A:351:THR:N	1:A:524:CYS:HB3	2.20	0.57
1:A:746:THR:HA	1:A:752:LEU:HD12	1.87	0.57
1:A:240:THR:O	1:A:244:ILE:HG12	2.06	0.56
1:A:891:ILE:HG22	1:A:906:VAL:HG12	1.87	0.56
1:A:1041:GLN:H	1:A:1041:GLN:NE2	2.03	0.56
1:A:744:LYS:HB2	1:A:744:LYS:HZ2	1.70	0.56
1:A:915:CYS:SG	1:A:920:LYS:HE2	2.46	0.56
1:A:760:SER:OG	1:A:762:GLN:HG2	2.07	0.55
1:A:181:VAL:HG12	1:A:185:MET:CE	2.37	0.55
1:A:887:THR:HG22	1:A:889:ALA:N	2.21	0.54
1:A:845:LEU:HD23	1:A:869:CYS:HB3	1.90	0.54
1:A:561:THR:HG21	1:A:565:ASN:ND2	2.23	0.54
1:A:158:ILE:CD1	1:A:717:LEU:HD13	2.38	0.54
1:A:807:LYS:H	1:A:807:LYS:CD	2.20	0.54
1:A:474:LEU:CD2	1:A:527:ILE:HG12	2.38	0.54
1:A:182:THR:HB	1:A:183:PRO:HD3	1.90	0.54
1:A:542:ARG:HD3	1:A:544:ARG:HH21	1.73	0.53
1:A:1000:LYS:HE3	1:A:1000:LYS:HA	1.89	0.53
1:A:804:MET:CE	1:A:812:TRP:HE3	2.21	0.53
1:A:741:MET:HE3	1:A:774:LEU:HD22	1.91	0.53
1:A:158:ILE:HD12	1:A:717:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:804:MET:HB3	1:A:810:PRO:HD2	1.90	0.53
1:A:245:LEU:HD21	1:A:272:LEU:HG	1.92	0.52
1:A:730:HIS:O	1:A:734:GLN:HG2	2.08	0.52
1:A:939:THR:HG21	3:A:2153:HOH:O	2.09	0.52
1:A:533:ARG:HG2	1:A:612:ALA:HB2	1.92	0.52
1:A:887:THR:HB	1:A:890:LYS:HG3	1.92	0.52
1:A:501:LYS:HZ2	1:A:501:LYS:HB3	1.73	0.52
1:A:914:LYS:HD2	1:A:956:GLU:HG2	1.91	0.52
1:A:158:ILE:HD13	1:A:717:LEU:HD13	1.92	0.51
1:A:903:LYS:HB2	1:A:906:VAL:HG23	1.92	0.51
1:A:1035:LEU:HB3	1:A:1043:THR:HG21	1.93	0.51
1:A:1026:LEU:O	1:A:1029:ILE:HG22	2.10	0.51
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.93	0.51
1:A:361:PHE:HB2	1:A:420:ILE:HD13	1.93	0.51
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.93	0.51
1:A:1029:ILE:O	1:A:1029:ILE:HD13	2.11	0.51
1:A:809:LYS:N	1:A:810:PRO:HD3	2.26	0.51
1:A:744:LYS:HB2	1:A:744:LYS:HZ3	1.74	0.50
1:A:364:LYS:HE2	1:A:411:ASN:OD1	2.12	0.50
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.42	0.50
1:A:1052:ARG:HH11	1:A:1052:ARG:HG2	1.75	0.50
1:A:597:LYS:HB2	1:A:603:ILE:HD12	1.93	0.49
1:A:379:LEU:HD13	1:A:435:CYS:SG	2.53	0.49
1:A:239:ASP:O	1:A:287:ILE:HG23	2.13	0.49
1:A:886:THR:HG22	1:A:887:THR:H	1.77	0.49
1:A:579:ARG:HB3	1:A:610:LEU:HD11	1.93	0.49
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.43	0.49
1:A:887:THR:HB	1:A:890:LYS:CG	2.42	0.49
1:A:853:SER:O	1:A:857:THR:HG23	2.12	0.48
1:A:354:LEU:HD22	1:A:529:LEU:HD21	1.96	0.48
1:A:235:VAL:HG11	1:A:244:ILE:HD13	1.95	0.48
1:A:150:PHE:HA	1:A:153:GLN:HE21	1.78	0.48
1:A:662:GLN:HE21	1:A:1030:LEU:HD22	1.77	0.48
1:A:741:MET:O	1:A:744:LYS:HG2	2.14	0.48
1:A:995:MET:O	1:A:1005:HIS:HB2	2.14	0.48
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.96	0.48
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.96	0.47
1:A:1041:GLN:H	1:A:1041:GLN:CD	2.17	0.47
1:A:467:LEU:O	1:A:476:ARG:HD2	2.14	0.47
1:A:547:MET:HE2	1:A:551:LEU:HB3	1.96	0.47
1:A:699:LEU:HB2	1:A:717:LEU:HG	1.96	0.47
1:A:180:LEU:C	1:A:183:PRO:HD2	2.35	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:179:ARG:NH2	1:A:679:ARG:HH22	2.13	0.47
1:A:925:VAL:O	1:A:929:VAL:HG23	2.15	0.47
1:A:162:VAL:HG12	1:A:714:ALA:HB1	1.97	0.47
1:A:935:TYR:O	1:A:939:THR:HG22	2.15	0.47
1:A:497:PHE:HB3	1:A:1042:LEU:HD22	1.96	0.47
1:A:479:GLU:HG2	1:A:519:LEU:HD13	1.96	0.46
1:A:410:TRP:O	1:A:412:VAL:HG23	2.15	0.46
1:A:1062:GLU:O	1:A:1066:LYS:HD3	2.15	0.46
1:A:728:MET:HE1	3:A:2107:HOH:O	2.13	0.46
1:A:181:VAL:HG12	1:A:185:MET:HE1	1.96	0.46
1:A:997:THR:HG23	1:A:1001:LYS:O	2.16	0.46
1:A:363:VAL:HG23	1:A:520:LEU:HD12	1.98	0.46
1:A:735:GLN:O	1:A:739:ILE:HD12	2.16	0.45
1:A:812:TRP:HA	1:A:831:ILE:HD13	1.98	0.45
1:A:271:VAL:HG23	1:A:282:VAL:HG11	1.98	0.45
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.98	0.45
1:A:863:CYS:HB3	1:A:927:ARG:HH11	1.80	0.45
1:A:225:HIS:NE2	1:A:304:HIS:HD2	2.15	0.45
1:A:888:ILE:HB	1:A:949:ASN:OD1	2.17	0.45
1:A:1052:ARG:HG3	1:A:1057:VAL:HG21	1.99	0.45
1:A:405:THR:HG23	1:A:407:GLU:O	2.17	0.45
1:A:749:ILE:CG2	1:A:752:LEU:HG	2.48	0.44
1:A:773:ASN:HA	1:A:776:ASN:ND2	2.31	0.44
1:A:773:ASN:HA	1:A:776:ASN:HD22	1.83	0.44
1:A:158:ILE:CD1	1:A:721:LEU:HD12	2.47	0.44
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	2.00	0.44
1:A:982:ARG:O	1:A:1078:LYS:HE2	2.18	0.44
1:A:545:ALA:HA	1:A:581:GLU:OE1	2.17	0.44
1:A:1052:ARG:O	1:A:1057:VAL:HG23	2.18	0.44
1:A:393:VAL:O	1:A:393:VAL:HG23	2.18	0.44
1:A:233:ILE:N	1:A:233:ILE:HD12	2.33	0.44
1:A:954:ILE:HD13	1:A:955:SER:N	2.32	0.44
1:A:941:VAL:O	1:A:1051:ILE:HD12	2.19	0.43
1:A:583:LEU:HD13	1:A:610:LEU:CD2	2.45	0.43
1:A:477:HIS:HB2	1:A:521:ASP:O	2.19	0.43
1:A:860:LEU:HD21	1:A:1015:LYS:HE2	2.01	0.43
1:A:744:LYS:NZ	1:A:744:LYS:CB	2.78	0.43
1:A:887:THR:CG2	1:A:950:ASP:HA	2.49	0.43
1:A:474:LEU:HD23	1:A:527:ILE:HG12	1.99	0.43
1:A:886:THR:HG22	1:A:887:THR:N	2.34	0.43
1:A:1035:LEU:HD12	1:A:1048:ILE:CD1	2.38	0.43
1:A:233:ILE:HG22	1:A:234:LYS:N	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:477:HIS:HD2	1:A:522:ASN:ND2	2.17	0.42
1:A:199:HIS:HB3	3:A:2014:HOH:O	2.19	0.42
1:A:1028:ILE:HD12	1:A:1051:ILE:HG23	2.02	0.42
1:A:544:ARG:HD2	1:A:577:HIS:O	2.19	0.42
1:A:772:GLU:HG2	1:A:798:ILE:CD1	2.43	0.42
1:A:696:PHE:HA	1:A:717:LEU:HD21	2.01	0.42
1:A:575:LEU:HD21	1:A:591:LYS:HB3	2.00	0.42
1:A:291:GLN:OE1	1:A:291:GLN:HA	2.18	0.42
1:A:389:TYR:O	1:A:392:GLN:HG2	2.19	0.42
1:A:809:LYS:O	1:A:834:HIS:HE1	2.02	0.42
1:A:370:ILE:O	1:A:370:ILE:HG23	2.20	0.42
1:A:782:SER:HA	1:A:793:ALA:O	2.20	0.42
1:A:547:MET:HE1	1:A:552:ARG:HA	2.02	0.42
1:A:705:GLN:NE2	1:A:875:LYS:H	2.17	0.42
1:A:381:VAL:HA	1:A:434:TYR:O	2.19	0.42
1:A:784:ARG:HG2	1:A:784:ARG:HH11	1.85	0.42
1:A:1031:PHE:CE2	1:A:1035:LEU:HD11	2.55	0.42
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.50	0.42
1:A:682:LEU:HD22	1:A:686:LEU:HD12	2.01	0.42
1:A:804:MET:CE	1:A:812:TRP:HB2	2.50	0.41
1:A:184:ARG:HD3	3:A:2009:HOH:O	2.19	0.41
1:A:222:ILE:O	1:A:222:ILE:HG13	2.20	0.41
1:A:497:PHE:O	1:A:498:ASN:HB3	2.20	0.41
1:A:354:LEU:HD22	1:A:529:LEU:HD11	2.03	0.41
1:A:373:LEU:HD23	1:A:406:GLU:N	2.35	0.41
1:A:376:THR:O	1:A:378:ASP:N	2.53	0.41
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.03	0.41
1:A:624:VAL:O	1:A:628:MET:HG2	2.20	0.41
1:A:235:VAL:HG11	1:A:244:ILE:HD12	2.03	0.41
1:A:543:VAL:O	1:A:544:ARG:C	2.59	0.41
1:A:235:VAL:HG12	1:A:236:SER:H	1.86	0.41
1:A:983:VAL:CG2	1:A:1075:CYS:SG	3.09	0.41
1:A:597:LYS:HB2	1:A:603:ILE:CD1	2.51	0.41
1:A:554:GLN:HA	1:A:554:GLN:NE2	2.36	0.41
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.56	0.41
1:A:1082:VAL:HB	3:A:2163:HOH:O	2.21	0.41
1:A:498:ASN:ND2	1:A:1042:LEU:HD23	2.36	0.40
1:A:939:THR:OG1	1:A:944:ILE:HG13	2.20	0.40
1:A:562:ASP:OD2	1:A:1052:ARG:HD3	2.22	0.40
1:A:762:GLN:H	1:A:762:GLN:CD	2.23	0.40
1:A:428:LEU:HD23	1:A:467:LEU:HA	2.03	0.40
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:VAL:HG12	1:A:185:MET:HE2	2.04	0.40
1:A:381:VAL:HG12	1:A:434:TYR:O	2.22	0.40
1:A:870:ILE:HG22	1:A:871:SER:O	2.22	0.40
1:A:270:PHE:CD2	1:A:307:LEU:HG	2.57	0.40
1:A:425:LYS:HE3	1:A:473:PHE:CZ	2.56	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	858/961 (89%)	799 (93%)	49 (6%)	10 (1%)	19   9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	ALA
1	A	524	CYS
1	A	534	PRO
1	A	542	ARG
1	A	251	LYS
1	A	778	ASN
1	A	896	VAL
1	A	374	PRO
1	A	490	LYS
1	A	376	THR

### 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	782/857 (91%)	751 (96%)	31 (4%)	42	36

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	VAL
1	A	355	TRP
1	A	356	ASP
1	A	374	PRO
1	A	487	LEU
1	A	501	LYS
1	A	522	ASN
1	A	523	TYR
1	A	533	ARG
1	A	610	LEU
1	A	626	LEU
1	A	682	LEU
1	A	717	LEU
1	A	744	LYS
1	A	758	ASP
1	A	762	GLN
1	A	791	LEU
1	A	807	LYS
1	A	836	ASP
1	A	843	LEU
1	A	845	LEU
1	A	883	LYS
1	A	905	GLU
1	A	907	LEU
1	A	913	GLU
1	A	954	ILE
1	A	1000	LYS
1	A	1026	LEU
1	A	1027	LEU
1	A	1029	ILE
1	A	1041	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	169	HIS

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Mol	Chain	Res	Type
1	A	199	HIS
1	A	218	ASN
1	A	299	ASN
1	A	304	HIS
1	A	391	GLN
1	A	459	GLN
1	A	477	HIS
1	A	483	HIS
1	A	522	ASN
1	A	554	GLN
1	A	565	ASN
1	A	601	GLN
1	A	658	HIS
1	A	705	GLN
1	A	737	GLN
1	A	762	GLN
1	A	769	GLN
1	A	773	ASN
1	A	776	ASN
1	A	778	ASN
1	A	834	HIS
1	A	951	ASN
1	A	1007	GLN
1	A	1041	GLN
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 ⓘ

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	KWT	A	1833	1	34,35,35	14.00	17 (50%)	52,57,57	20.08	20 (38%)

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	KWT	A	1833	1	-	0/7/75/75	0/0/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1833	KWT	O5-C19	79.02	3.09	1.35
2	A	1833	KWT	C9-C4	11.15	1.64	1.53
2	A	1833	KWT	C11-C8	8.60	1.61	1.51
2	A	1833	KWT	C9-C8	7.51	1.63	1.52
2	A	1833	KWT	O1-C2	5.65	1.43	1.34
2	A	1833	KWT	C15-C7	4.57	1.59	1.51
2	A	1833	KWT	C3-C2	3.77	1.59	1.49
2	A	1833	KWT	C8-C7	3.68	1.41	1.35
2	A	1833	KWT	C5-C6	3.55	1.54	1.49
2	A	1833	KWT	C10-C9	3.25	1.58	1.54
2	A	1833	KWT	C3-C4	3.19	1.42	1.38
2	A	1833	KWT	C7-C6	3.13	1.54	1.47
2	A	1833	KWT	C12-C11	2.71	1.57	1.52
2	A	1833	KWT	O6-C21	2.68	1.41	1.35
2	A	1833	KWT	C23-C1	2.58	1.56	1.50
2	A	1833	KWT	C9-C1	2.53	1.58	1.54
2	A	1833	KWT	C12-C13	2.02	1.57	1.54



All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1833	KWT	C19-O5-C5	-119.59	81.40	106.42
2	A	1833	KWT	O5-C19-C3	-74.23	72.71	110.60
2	A	1833	KWT	C3-C4-C5	25.54	124.84	107.59
2	A	1833	KWT	C9-C4-C3	-12.28	117.73	124.16
2	A	1833	KWT	C19-C3-C4	11.24	132.14	110.51
2	A	1833	KWT	C16-C15-C13	-6.74	100.07	104.37
2	A	1833	KWT	C4-C9-C8	6.62	116.49	109.15
2	A	1833	KWT	C10-C9-C8	-4.20	103.31	108.72
2	A	1833	KWT	C11-O6-C21	3.71	123.05	117.13
2	A	1833	KWT	C16-C17-C18	-3.31	102.25	105.67
2	A	1833	KWT	C10-C9-C4	-3.27	107.42	111.92
2	A	1833	KWT	O3-C6-C5	-2.92	117.53	121.92
2	A	1833	KWT	C12-C13-C15	-2.69	103.02	110.82
2	A	1833	KWT	O1-C2-C3	-2.63	115.70	118.04
2	A	1833	KWT	C14-C13-C15	2.58	117.24	112.01
2	A	1833	KWT	C1-O1-C2	2.53	125.89	119.40
2	A	1833	KWT	C17-C18-C13	2.32	110.94	108.60
2	A	1833	KWT	C5-C6-C7	2.32	119.86	118.14
2	A	1833	KWT	C14-C13-C18	2.30	109.85	105.21
2	A	1833	KWT	C4-C5-C6	2.15	124.36	122.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	872/961 (90%)	0.42	50 (5%) 23 22	24, 47, 81, 101	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	LYS	6.5
1	A	522	ASN	6.5
1	A	266	ASN	5.6
1	A	777	LEU	5.3
1	A	249	PHE	5.2
1	A	253	ALA	5.1
1	A	823	LEU	4.9
1	A	541	ASP	4.8
1	A	898	ASN	4.7
1	A	375	ARG	4.7
1	A	143	ALA	4.6
1	A	527	ILE	4.4
1	A	529	LEU	3.9
1	A	252	MET	3.9
1	A	268	ARG	3.7
1	A	918	GLU	3.7
1	A	542	ARG	3.7
1	A	533	ARG	3.6
1	A	267	GLU	3.6
1	A	895	THR	3.6
1	A	525	HIS	3.6
1	A	354	LEU	3.3
1	A	307	LEU	3.1
1	A	488	SER	3.0
1	A	979	ASN	2.9
1	A	523	TYR	2.8
1	A	233	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	998	SER	2.8
1	A	535	THR	2.7
1	A	235	VAL	2.5
1	A	248	PHE	2.5
1	A	528	ALA	2.5
1	A	377	ALA	2.5
1	A	919	GLU	2.5
1	A	359	ARG	2.4
1	A	376	THR	2.4
1	A	270	PHE	2.3
1	A	245	LEU	2.3
1	A	351	THR	2.3
1	A	992	LEU	2.3
1	A	211	LEU	2.3
1	A	370	ILE	2.2
1	A	997	THR	2.2
1	A	282	VAL	2.2
1	A	534	PRO	2.2
1	A	148	LEU	2.1
1	A	524	CYS	2.1
1	A	353	SER	2.1
1	A	281	LEU	2.0
1	A	949	ASN	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 ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	KWT	A	1833	31/31	0.20	3.45	34,39,59,63	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.