



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:33 am GMT

PDB ID : 1E8Z  
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 : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

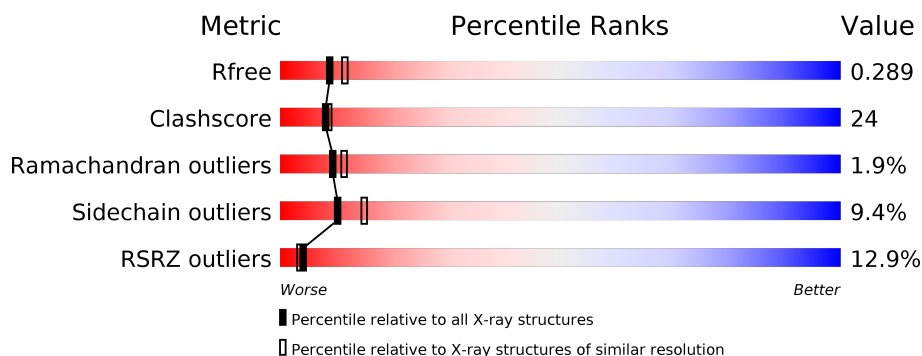
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	966	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	STU	A	3001	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6876 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.

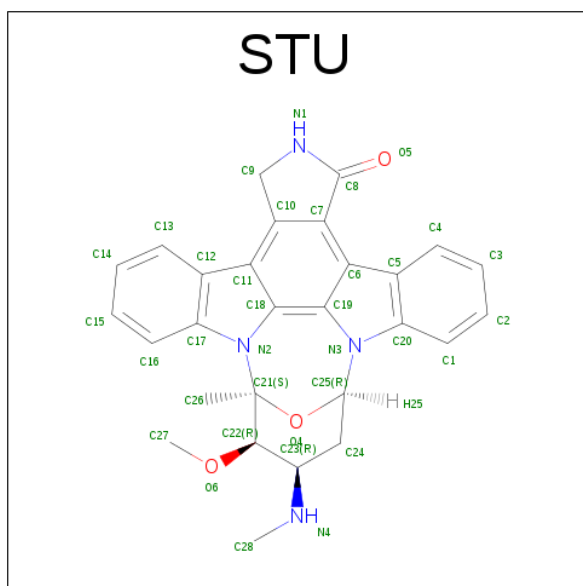
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	839	6801	4367	1162	1237	35	0	0	0

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 STAUROSPORINE (three-letter code: STU) (formula:  $C_{28}H_{26}N_4O_3$ ).

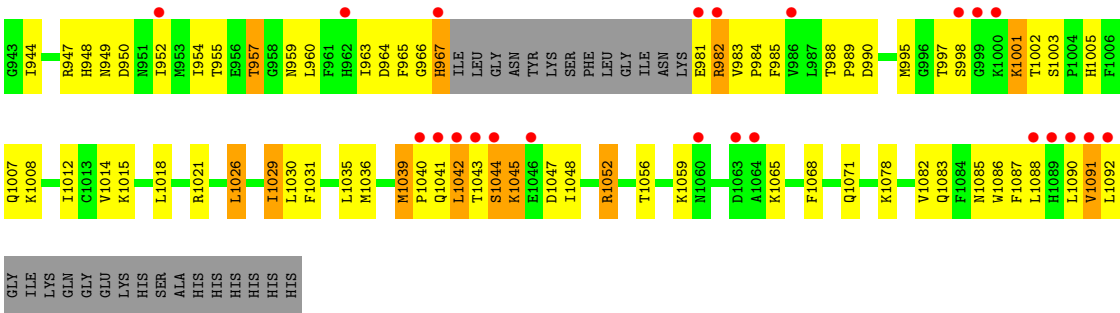


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	35	28	4	3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.49Å 66.99Å 104.11Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	60.84 – 2.40 26.68 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.9 (60.84-2.40) 88.0 (26.68-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 2.42Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.232 , 0.291 0.232 , 0.289	Depositor DCC
$R_{free}$ test set	1935 reflections (5.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.5	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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](#)

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

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	0.68	0/6946	0.73	0/9393

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	720	TYR	Sidechain

### 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	6801	0	6845	323	0
2	A	35	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	40	0	0	2	0
All	All	6876	0	6871	323	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 24.

All (323) 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:629:GLN:HG2	1:A:1029:ILE:HG13	1.41	1.01
1:A:149:ALA:HA	1:A:152:ARG:HD3	1.43	1.00
1:A:381:VAL:HG23	1:A:435:CYS:HB3	1.44	0.98
1:A:981:GLU:N	1:A:982:ARG:HH21	1.62	0.97
1:A:750:LYS:HE2	1:A:809:LYS:H	1.30	0.94
1:A:887:THR:HG21	1:A:950:ASP:HA	1.50	0.93
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.18	0.90
1:A:240:THR:HG22	1:A:242:GLY:H	1.39	0.87
1:A:1008:LYS:O	1:A:1012:ILE:HG13	1.74	0.85
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.57	0.84
1:A:202:VAL:HG12	1:A:203:THR:N	1.93	0.83
1:A:860:LEU:HD11	1:A:1015:LYS:HG2	1.63	0.81
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.62	0.81
1:A:981:GLU:C	1:A:982:ARG:HE	1.84	0.80
1:A:887:THR:HG22	1:A:889:ALA:H	1.46	0.80
1:A:379:LEU:HD13	1:A:380:THR:H	1.48	0.79
1:A:217:ASN:ND2	1:A:219:CYS:HB3	1.98	0.79
1:A:750:LYS:HA	1:A:809:LYS:HG3	1.63	0.79
1:A:836:ASP:O	1:A:875:LYS:HA	1.83	0.78
1:A:561:THR:HG22	1:A:591:LYS:NZ	2.00	0.77
1:A:750:LYS:HE2	1:A:809:LYS:N	2.00	0.77
1:A:380:THR:O	1:A:435:CYS:HB2	1.86	0.76
1:A:935:TYR:O	1:A:939:THR:HG22	1.87	0.75
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.69	0.75
1:A:1044:SER:O	1:A:1045:LYS:HG3	1.86	0.74
1:A:887:THR:CG2	1:A:950:ASP:HA	2.17	0.74
1:A:568:THR:HG22	1:A:570:GLU:H	1.52	0.74
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.03	0.73
1:A:361:PHE:HB2	1:A:420:ILE:HD13	1.70	0.73
1:A:379:LEU:HD13	1:A:380:THR:N	2.05	0.71
1:A:807:LYS:HD2	1:A:808:LYS:H	1.55	0.70
1:A:848:LEU:HD12	1:A:851:MET:HE1	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:PHE:O	1:A:967:HIS:N	2.26	0.69
1:A:245:LEU:O	1:A:248:PHE:HB3	1.92	0.68
1:A:891:ILE:HG22	1:A:906:VAL:HG12	1.73	0.68
1:A:371:PRO:HG2	1:A:511:GLU:O	1.93	0.68
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.29	0.68
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.41	0.68
1:A:791:LEU:HD12	1:A:828:ILE:HD11	1.76	0.67
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.74	0.67
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.76	0.67
1:A:277:ARG:CZ	1:A:791:LEU:HD23	2.23	0.67
1:A:202:VAL:CG1	1:A:203:THR:N	2.57	0.67
1:A:486:GLN:HG2	1:A:487:ILE:H	1.58	0.67
1:A:825:ASN:HD22	1:A:825:ASN:H	1.42	0.67
1:A:981:GLU:N	1:A:982:ARG:NH2	2.40	0.67
1:A:625:GLY:O	1:A:629:GLN:HG3	1.96	0.66
1:A:182:THR:HB	1:A:183:PRO:HD3	1.77	0.66
1:A:213:LYS:NZ	1:A:214:LYS:HB2	2.11	0.66
1:A:558:ILE:O	1:A:561:THR:HB	1.96	0.66
1:A:202:VAL:HG12	1:A:203:THR:H	1.59	0.66
1:A:617:TRP:CE2	1:A:643:ILE:HD12	2.31	0.66
1:A:202:VAL:HG13	1:A:289:ASN:O	1.96	0.65
1:A:597:LYS:HB2	1:A:603:ILE:HD13	1.76	0.65
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.79	0.65
1:A:888:ILE:HD13	1:A:952:ILE:HG22	1.78	0.65
1:A:1042:LEU:H	1:A:1042:LEU:HD13	1.60	0.65
1:A:202:VAL:CG1	1:A:203:THR:H	2.10	0.64
1:A:1002:THR:HG22	1:A:1003:SER:H	1.63	0.64
1:A:375:ARG:HG2	1:A:376:ASN:H	1.61	0.64
1:A:373:LEU:H	1:A:374:PRO:HD2	1.63	0.64
1:A:569:ALA:O	1:A:573:GLU:HG3	1.98	0.64
1:A:833:LYS:HG3	1:A:834:HIS:N	2.13	0.64
1:A:270:PHE:HB3	1:A:307:LEU:HD11	1.79	0.63
1:A:739:ILE:HG22	1:A:878:MET:HE1	1.80	0.63
1:A:561:THR:HG22	1:A:591:LYS:HZ1	1.62	0.62
1:A:825:ASN:ND2	1:A:825:ASN:H	1.97	0.62
1:A:804:MET:HE1	1:A:812:TRP:HB2	1.80	0.62
1:A:498:ASN:HB3	1:A:1041:GLN:NE2	2.13	0.62
1:A:373:LEU:H	1:A:374:PRO:CD	2.13	0.62
1:A:435:CYS:SG	1:A:461:LEU:HD11	2.40	0.61
1:A:181:VAL:O	1:A:185:MET:HG3	2.00	0.61
1:A:395:CYS:HB2	1:A:418:ILE:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ALA:O	1:A:152:ARG:HB2	2.01	0.61
1:A:561:THR:CG2	1:A:565:ASN:HB3	2.30	0.60
1:A:622:LEU:HD21	1:A:651:LEU:CD2	2.31	0.60
1:A:1043:THR:C	1:A:1045:LYS:H	2.04	0.59
1:A:148:GLN:O	1:A:152:ARG:HG3	2.02	0.59
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.68	0.59
1:A:983:VAL:HG23	1:A:1082:VAL:HG21	1.85	0.59
1:A:903:LYS:HB2	1:A:906:VAL:HG23	1.85	0.58
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.30	0.58
1:A:807:LYS:HD2	1:A:807:LYS:N	2.19	0.58
1:A:221:PHE:CE2	1:A:234:LYS:HG2	2.38	0.57
1:A:287:ILE:HD12	1:A:288:LYS:N	2.19	0.57
1:A:432:GLN:OE1	1:A:501:LYS:NZ	2.37	0.57
1:A:629:GLN:HG2	1:A:1029:ILE:CG1	2.26	0.57
1:A:804:MET:HB2	1:A:810:PRO:HB2	1.85	0.57
1:A:291:GLN:HA	1:A:291:GLN:OE1	2.03	0.57
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.40	0.57
1:A:690:ARG:NH1	1:A:789:PRO:HG2	2.20	0.57
1:A:836:ASP:H	1:A:875:LYS:HB3	1.69	0.57
1:A:1042:LEU:N	1:A:1042:LEU:HD13	2.20	0.57
1:A:168:VAL:HG13	1:A:170:ASP:H	1.70	0.57
1:A:874:ASP:O	1:A:875:LYS:HB2	2.03	0.57
1:A:1036:MET:HA	1:A:1042:LEU:HD11	1.86	0.57
1:A:277:ARG:NH2	1:A:791:LEU:HD23	2.20	0.57
1:A:768:LYS:O	1:A:772:GLU:HG2	2.04	0.56
1:A:165:VAL:O	1:A:165:VAL:HG12	2.06	0.56
1:A:370:ILE:HD12	1:A:372:VAL:O	2.05	0.56
1:A:1042:LEU:HD22	1:A:1042:LEU:O	2.05	0.56
1:A:734:GLN:HE21	1:A:734:GLN:HA	1.69	0.56
1:A:739:ILE:O	1:A:743:GLN:HG3	2.06	0.56
1:A:561:THR:HG22	1:A:591:LYS:HZ2	1.71	0.56
1:A:845:LEU:O	1:A:849:ARG:HG3	2.06	0.56
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.70	0.55
1:A:1002:THR:HG22	1:A:1003:SER:N	2.21	0.55
1:A:787:TYR:OH	1:A:830:ILE:HG12	2.05	0.55
1:A:220:ILE:HD12	1:A:287:ILE:HD13	1.87	0.55
1:A:583:LEU:HD22	1:A:610:LEU:CD2	2.37	0.55
1:A:840:GLN:HG2	1:A:1039:MET:HE2	1.89	0.55
1:A:804:MET:CE	1:A:812:TRP:HB2	2.37	0.55
1:A:927:ARG:HE	1:A:959:ASN:HD22	1.54	0.55
1:A:1052:ARG:HH11	1:A:1052:ARG:HG2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:GLY:HA2	1:A:875:LYS:HE3	1.90	0.54
1:A:745:VAL:HG21	1:A:774:LEU:HD11	1.90	0.54
1:A:791:LEU:HD12	1:A:828:ILE:CD1	2.37	0.54
1:A:627:THR:HG21	1:A:648:LEU:CD2	2.37	0.54
1:A:410:TRP:O	1:A:412:VAL:HG23	2.07	0.54
1:A:662:GLN:NE2	1:A:1030:LEU:HD22	2.22	0.54
1:A:207:LEU:HA	1:A:294:ARG:NH1	2.23	0.54
1:A:988:THR:HB	1:A:989:PRO:CD	2.38	0.54
1:A:370:ILE:HD13	1:A:371:PRO:N	2.23	0.54
1:A:149:ALA:HA	1:A:152:ARG:HH11	1.72	0.53
1:A:178:ARG:HH11	1:A:178:ARG:HG3	1.73	0.53
1:A:653:ASP:OD1	3:A:2021:HOH:O	2.19	0.53
1:A:743:GLN:O	1:A:747:LEU:HG	2.09	0.53
1:A:848:LEU:HA	1:A:851:MET:HE2	1.89	0.53
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	2.24	0.53
1:A:561:THR:HG23	1:A:565:ASN:HB3	1.91	0.53
1:A:805:ALA:O	1:A:806:SER:O	2.27	0.53
1:A:233:ILE:N	1:A:233:ILE:HD12	2.22	0.53
1:A:753:SER:HB2	1:A:809:LYS:NZ	2.24	0.52
1:A:235:VAL:HG11	1:A:244:ILE:HD11	1.92	0.52
1:A:697:TRP:HH2	1:A:739:ILE:HD13	1.75	0.52
1:A:483:HIS:HD2	3:A:2013:HOH:O	1.92	0.52
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.10	0.52
1:A:361:PHE:HB2	1:A:420:ILE:CD1	2.39	0.52
1:A:949:ASN:N	1:A:1083:GLN:HE22	1.97	0.52
1:A:240:THR:HG22	1:A:242:GLY:N	2.17	0.52
1:A:606:LYS:HA	1:A:609:GLN:OE1	2.11	0.51
1:A:170:ASP:C	1:A:170:ASP:OD1	2.48	0.51
1:A:583:LEU:HD13	1:A:610:LEU:HD22	1.92	0.51
1:A:947:ARG:NH2	1:A:963:ILE:O	2.44	0.51
1:A:905:GLU:HB3	1:A:909:HIS:NE2	2.25	0.51
1:A:251:LYS:HB3	1:A:252:MET:SD	2.51	0.51
1:A:758:ASP:CG	1:A:759:VAL:H	2.13	0.51
1:A:359:ARG:HG3	1:A:360:LYS:N	2.26	0.51
1:A:622:LEU:HD21	1:A:651:LEU:HD21	1.93	0.51
1:A:219:CYS:SG	1:A:234:LYS:HB3	2.51	0.51
1:A:763:VAL:HG13	1:A:764:ILE:N	2.25	0.51
1:A:887:THR:HG21	1:A:950:ASP:OD1	2.11	0.51
1:A:1021:ARG:HE	1:A:1056:THR:CG2	2.25	0.50
1:A:699:LEU:HD22	1:A:713:PHE:HD2	1.76	0.50
1:A:831:ILE:HG13	1:A:881:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.94	0.50
1:A:375:ARG:HG2	1:A:376:ASN:N	2.25	0.50
1:A:997:THR:HG23	1:A:1001:LYS:HB3	1.94	0.50
1:A:749:ILE:HG12	1:A:767:LEU:HD23	1.93	0.50
1:A:963:ILE:HD12	1:A:964:ASP:OD1	2.10	0.50
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.92	0.50
1:A:568:THR:HG22	1:A:569:ALA:N	2.25	0.50
1:A:997:THR:HG22	1:A:998:SER:N	2.26	0.50
1:A:600:GLN:CB	1:A:603:ILE:HD12	2.41	0.50
1:A:983:VAL:CG1	1:A:985:PHE:O	2.59	0.50
1:A:246:GLN:C	1:A:248:PHE:H	2.16	0.49
1:A:435:CYS:SG	1:A:461:LEU:CD1	3.00	0.49
1:A:848:LEU:HD12	1:A:851:MET:CE	2.42	0.49
1:A:562:ASP:OD1	1:A:1052:ARG:NH1	2.45	0.49
1:A:379:LEU:HD13	1:A:380:THR:HG22	1.94	0.49
1:A:214:LYS:HZ2	1:A:300:GLY:HA2	1.76	0.49
1:A:760:SER:O	1:A:763:VAL:HG12	2.12	0.49
1:A:278:ASP:OD1	1:A:784:ARG:NH2	2.45	0.49
1:A:1086:TRP:HH2	1:A:1090:LEU:HB2	1.78	0.49
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.13	0.49
1:A:893:GLN:HA	1:A:897:GLY:O	2.13	0.49
1:A:807:LYS:HD2	1:A:808:LYS:N	2.27	0.48
1:A:955:THR:OG1	1:A:957:THR:HG22	2.12	0.48
1:A:270:PHE:HB3	1:A:307:LEU:CD1	2.41	0.48
1:A:373:LEU:HD11	1:A:404:PHE:O	2.12	0.48
1:A:739:ILE:HG13	1:A:740:GLU:N	2.27	0.48
1:A:932:CYS:HA	1:A:960:LEU:HD22	1.94	0.48
1:A:197:ALA:HA	1:A:689:LYS:HE3	1.95	0.48
1:A:739:ILE:HG22	1:A:878:MET:CE	2.42	0.48
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.14	0.48
1:A:1043:THR:HB	1:A:1047:ASP:H	1.78	0.48
1:A:836:ASP:N	1:A:875:LYS:HB3	2.29	0.48
1:A:1026:LEU:HD22	1:A:1030:LEU:HG	1.95	0.48
1:A:896:VAL:CG2	1:A:903:LYS:HG3	2.43	0.48
1:A:1086:TRP:O	1:A:1087:PHE:CD1	2.67	0.48
1:A:149:ALA:CB	1:A:152:ARG:HH11	2.27	0.48
1:A:1052:ARG:NH1	1:A:1052:ARG:HG2	2.28	0.47
1:A:244:ILE:HA	1:A:247:SER:OG	2.14	0.47
1:A:287:ILE:HA	1:A:290:PHE:HD1	1.79	0.47
1:A:862:LEU:CD2	1:A:862:LEU:N	2.77	0.47
1:A:997:THR:HG22	1:A:998:SER:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:SER:C	1:A:1045:LYS:HG3	2.34	0.47
1:A:1085:ASN:O	1:A:1087:PHE:N	2.47	0.47
1:A:395:CYS:HB2	1:A:418:ILE:CD1	2.43	0.47
1:A:600:GLN:HG3	1:A:603:ILE:HD12	1.96	0.47
1:A:202:VAL:HG11	1:A:285:THR:HG21	1.96	0.47
1:A:568:THR:CG2	1:A:569:ALA:N	2.77	0.47
1:A:948:HIS:NE2	1:A:950:ASP:HB2	2.30	0.47
1:A:643:ILE:HG13	1:A:644:ALA:N	2.29	0.47
1:A:213:LYS:HZ3	1:A:214:LYS:HB2	1.79	0.47
1:A:983:VAL:CG2	1:A:1082:VAL:HG21	2.44	0.47
1:A:213:LYS:HD3	1:A:214:LYS:N	2.30	0.47
1:A:667:VAL:HG12	1:A:667:VAL:O	2.14	0.47
1:A:210:TYR:OH	1:A:856:GLU:HG3	2.15	0.46
1:A:1014:VAL:O	1:A:1018:LEU:HG	2.15	0.46
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.80	0.46
1:A:804:MET:HE3	1:A:810:PRO:HB2	1.96	0.46
1:A:796:LEU:HG	1:A:815:PHE:CE2	2.50	0.46
1:A:983:VAL:HG13	1:A:984:PRO:HD2	1.97	0.46
1:A:1021:ARG:NH2	1:A:1056:THR:HG23	2.31	0.46
1:A:188:VAL:O	1:A:191:ARG:HG2	2.16	0.46
1:A:954:ILE:HA	1:A:959:ASN:O	2.14	0.46
1:A:576:TRP:O	1:A:579:ARG:HG2	2.14	0.46
1:A:1021:ARG:NE	1:A:1056:THR:CG2	2.78	0.46
1:A:276:GLY:HA2	1:A:819:ASP:CG	2.35	0.46
1:A:602:GLU:O	1:A:606:LYS:HG3	2.16	0.46
1:A:762:GLN:O	1:A:766:GLN:HG3	2.15	0.46
1:A:1042:LEU:HD23	1:A:1048:ILE:HD11	1.97	0.45
1:A:1021:ARG:HH21	1:A:1056:THR:HG23	1.81	0.45
1:A:772:GLU:OE2	1:A:798:ILE:HG21	2.15	0.45
1:A:320:LYS:HG3	1:A:320:LYS:H	1.39	0.45
1:A:424:PRO:HG2	1:A:427:ALA:HB2	1.97	0.45
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.98	0.45
1:A:1008:LYS:HG3	1:A:1012:ILE:HD11	1.98	0.45
1:A:1043:THR:C	1:A:1045:LYS:N	2.70	0.45
1:A:217:ASN:HD22	1:A:219:CYS:HB3	1.76	0.45
1:A:841:ASP:O	1:A:845:LEU:HD22	2.17	0.45
1:A:697:TRP:CH2	1:A:739:ILE:HD13	2.51	0.45
1:A:983:VAL:CG2	1:A:1078:LYS:HG2	2.47	0.44
1:A:1035:LEU:HB3	1:A:1042:LEU:HG	1.99	0.44
1:A:1039:MET:N	1:A:1039:MET:CE	2.80	0.44
1:A:232:THR:C	1:A:233:ILE:HD12	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LEU:CD2	1:A:305:VAL:HG21	2.48	0.44
1:A:390:GLY:C	1:A:392:GLN:H	2.20	0.44
1:A:1001:LYS:HG3	1:A:1002:THR:H	1.82	0.44
1:A:364:LYS:O	1:A:518:ILE:HA	2.18	0.44
1:A:807:LYS:N	1:A:807:LYS:CD	2.79	0.44
1:A:891:ILE:HG22	1:A:906:VAL:CG1	2.46	0.44
1:A:921:PHE:O	1:A:925:VAL:HG23	2.18	0.44
1:A:614:ARG:CZ	1:A:643:ILE:HG22	2.48	0.43
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.99	0.43
1:A:1001:LYS:NZ	1:A:1001:LYS:HB2	2.33	0.43
1:A:1014:VAL:HG11	1:A:1065:LYS:HD2	2.01	0.43
1:A:431:LEU:O	1:A:463:TYR:HA	2.18	0.43
1:A:750:LYS:HA	1:A:809:LYS:CG	2.42	0.43
1:A:756:LYS:HE3	1:A:757:TYR:N	2.34	0.43
1:A:929:VAL:HG22	1:A:995:MET:HG2	2.00	0.43
1:A:622:LEU:HD22	1:A:650:SER:OG	2.19	0.43
1:A:146:GLU:HB3	1:A:319:ARG:HH22	1.84	0.43
1:A:498:ASN:HB3	1:A:1041:GLN:HE22	1.82	0.43
1:A:312:ASP:HA	1:A:313:PRO:HD2	1.89	0.43
1:A:825:ASN:N	1:A:825:ASN:ND2	2.66	0.43
1:A:851:MET:HE2	1:A:851:MET:HB2	1.88	0.43
1:A:1043:THR:O	1:A:1045:LYS:N	2.50	0.43
1:A:214:LYS:NZ	1:A:297:LEU:HA	2.34	0.43
1:A:235:VAL:HG11	1:A:244:ILE:CD1	2.49	0.43
1:A:1021:ARG:NE	1:A:1056:THR:HG23	2.33	0.42
1:A:701:SER:O	1:A:705:GLN:HG3	2.19	0.42
1:A:1026:LEU:HD22	1:A:1026:LEU:O	2.18	0.42
1:A:357:CYS:SG	1:A:359:ARG:HB3	2.59	0.42
1:A:635:PHE:O	1:A:641:ARG:HD2	2.19	0.42
1:A:667:VAL:O	1:A:667:VAL:CG1	2.67	0.42
1:A:752:LEU:O	1:A:753:SER:CB	2.65	0.42
1:A:745:VAL:CG2	1:A:774:LEU:HD11	2.49	0.42
1:A:935:TYR:O	1:A:939:THR:CG2	2.60	0.42
1:A:1086:TRP:C	1:A:1087:PHE:CD1	2.93	0.42
1:A:995:MET:O	1:A:1005:HIS:HB2	2.19	0.42
1:A:939:THR:OG1	1:A:944:ILE:HG13	2.20	0.42
1:A:202:VAL:CG1	1:A:285:THR:HG21	2.49	0.42
1:A:382:PHE:CE1	1:A:434:TYR:HB2	2.55	0.42
1:A:988:THR:OG1	1:A:990:ASP:OD1	2.24	0.42
1:A:862:LEU:HD22	1:A:862:LEU:N	2.35	0.42
1:A:888:ILE:CG2	1:A:949:ASN:OD1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.50	0.42
1:A:486:GLN:HG2	1:A:487:ILE:N	2.31	0.42
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.54	0.42
1:A:210:TYR:O	1:A:213:LYS:HD2	2.20	0.42
1:A:246:GLN:C	1:A:248:PHE:N	2.73	0.42
1:A:734:GLN:HE22	1:A:780:PRO:HB3	1.85	0.41
1:A:918:GLU:O	1:A:922:GLN:HG2	2.20	0.41
1:A:473:PHE:HB3	1:A:527:ILE:HD12	2.02	0.41
1:A:486:GLN:CG	1:A:487:ILE:H	2.31	0.41
1:A:547:MET:HA	1:A:548:PRO:HD3	1.81	0.41
1:A:736:VAL:O	1:A:740:GLU:HB2	2.20	0.41
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.56	0.41
1:A:627:THR:HG21	1:A:648:LEU:HD21	2.02	0.41
1:A:890:LYS:HB2	1:A:890:LYS:HE3	1.80	0.41
1:A:420:ILE:HA	1:A:420:ILE:HD13	1.90	0.41
1:A:477:ARG:HA	1:A:520:LEU:HB3	2.03	0.41
1:A:1031:PHE:O	1:A:1035:LEU:HG	2.19	0.41
1:A:149:ALA:CA	1:A:152:ARG:HH11	2.33	0.41
1:A:278:ASP:OD1	1:A:784:ARG:CZ	2.69	0.41
1:A:214:LYS:HZ3	1:A:297:LEU:HA	1.86	0.41
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.88	0.41
1:A:237:PRO:HA	1:A:287:ILE:CD1	2.51	0.41
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.28	0.41
1:A:758:ASP:CG	1:A:759:VAL:N	2.73	0.41
1:A:1021:ARG:HE	1:A:1056:THR:HG23	1.86	0.41
1:A:237:PRO:HA	1:A:287:ILE:HD11	2.03	0.41
1:A:361:PHE:C	1:A:361:PHE:CD2	2.93	0.41
1:A:617:TRP:CZ2	1:A:643:ILE:HD12	2.56	0.41
1:A:184:ARG:HH11	1:A:184:ARG:HB2	1.85	0.41
1:A:242:GLY:O	1:A:245:LEU:HB2	2.20	0.41
1:A:357:CYS:O	1:A:421:LYS:HB2	2.20	0.41
1:A:851:MET:CE	1:A:938:ALA:HB1	2.45	0.41
1:A:988:THR:HB	1:A:989:PRO:HD2	2.02	0.41
1:A:614:ARG:HD3	1:A:646:GLN:HE22	1.85	0.41
1:A:373:LEU:N	1:A:374:PRO:CD	2.81	0.41
1:A:750:LYS:CE	1:A:808:LYS:HB3	2.50	0.41
1:A:223:VAL:HB	1:A:304:HIS:CD2	2.56	0.40
1:A:739:ILE:CG1	1:A:740:GLU:N	2.84	0.40
1:A:887:THR:HG22	1:A:888:ILE:N	2.36	0.40
1:A:172:GLU:CD	1:A:673:HIS:CD2	2.95	0.40
1:A:390:GLY:C	1:A:392:GLN:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ASP:OD1	1:A:646:GLN:OE1	2.39	0.40
1:A:806:SER:HB2	1:A:810:PRO:HG2	2.02	0.40
1:A:1068:PHE:O	1:A:1071:GLN:HB2	2.22	0.40
1:A:896:VAL:HG22	1:A:903:LYS:HG3	2.02	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	821/966 (85%)	741 (90%)	64 (8%)	16 (2%)	9	11

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	615	GLU
1	A	753	SER
1	A	806	SER
1	A	898	ASN
1	A	966	GLY
1	A	1040	PRO
1	A	1088	LEU
1	A	373	LEU
1	A	754	ALA
1	A	1091	VAL
1	A	374	PRO
1	A	1044	SER
1	A	1045	LYS
1	A	371	PRO
1	A	759	VAL

### 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	754/864 (87%)	683 (91%)	71 (9%)	10	15

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	146	GLU
1	A	185	MET
1	A	207	LEU
1	A	213	LYS
1	A	226	ARG
1	A	252	MET
1	A	269	ASP
1	A	277	ARG
1	A	281	LEU
1	A	291	GLN
1	A	309	THR
1	A	320	LYS
1	A	361	PHE
1	A	370	ILE
1	A	373	LEU
1	A	374	PRO
1	A	379	LEU
1	A	393	VAL
1	A	395	CYS
1	A	404	PHE
1	A	435	CYS
1	A	476	ARG
1	A	487	ILE
1	A	498	ASN
1	A	512	ASN
1	A	544	ARG
1	A	554	GLN
1	A	555	LEU
1	A	561	THR

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Mol	Chain	Res	Type
1	A	562	ASP
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	646	GLN
1	A	647	LYS
1	A	682	LEU
1	A	717	LEU
1	A	734	GLN
1	A	753	SER
1	A	756	LYS
1	A	757	TYR
1	A	791	LEU
1	A	796	LEU
1	A	802	LYS
1	A	804	MET
1	A	806	SER
1	A	807	LYS
1	A	825	ASN
1	A	836	ASP
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	883	LYS
1	A	899	THR
1	A	907	LEU
1	A	915	SER
1	A	926	GLU
1	A	957	THR
1	A	967	HIS
1	A	982	ARG
1	A	1001	LYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1039	MET
1	A	1042	LEU
1	A	1052	ARG
1	A	1059	LYS
1	A	1091	VAL
1	A	1092	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	225	HIS
1	A	304	HIS
1	A	483	HIS
1	A	565	ASN
1	A	646	GLN
1	A	662	GLN
1	A	734	GLN
1	A	743	GLN
1	A	766	GLN
1	A	773	ASN
1	A	825	ASN
1	A	908	ASN
1	A	959	ASN
1	A	1041	GLN
1	A	1083	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	STU	A	3001	-	29,42,42	2.96	18 (62%)	27,68,68	1.18	2 (7%)

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	STU	A	3001	-	-	0/4/42/42	0/0/8/8

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	STU	C8-N1	-4.64	1.31	1.35
2	A	3001	STU	C3-C4	2.46	1.42	1.36
2	A	3001	STU	C11-C18	2.59	1.46	1.42
2	A	3001	STU	C15-C16	2.75	1.43	1.36
2	A	3001	STU	C4-C5	2.79	1.46	1.41
2	A	3001	STU	C1-C20	2.86	1.46	1.41
2	A	3001	STU	C2-C1	2.90	1.43	1.36
2	A	3001	STU	C14-C13	2.96	1.43	1.36
2	A	3001	STU	C19-C18	2.98	1.49	1.42
2	A	3001	STU	O6-C22	2.99	1.48	1.42
2	A	3001	STU	C6-C19	3.14	1.47	1.42
2	A	3001	STU	C10-C11	3.42	1.49	1.42
2	A	3001	STU	C13-C12	3.60	1.48	1.41
2	A	3001	STU	C16-C17	3.84	1.49	1.41
2	A	3001	STU	C26-C21	4.16	1.56	1.51
2	A	3001	STU	C7-C6	4.75	1.50	1.43
2	A	3001	STU	C24-C25	4.95	1.59	1.51
2	A	3001	STU	C22-C23	5.34	1.58	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	STU	C9-C10-C7	-3.19	106.76	109.61
2	A	3001	STU	C16-C17-C12	-2.18	117.58	120.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	839/966 (86%)	0.63	108 (12%) 4 3	25, 51, 94, 119	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1089	HIS	9.5
1	A	1090	LEU	6.8
1	A	823	LEU	6.7
1	A	751	SER	6.5
1	A	216	ALA	6.1
1	A	377	THR	6.0
1	A	322	GLU	5.9
1	A	1091	VAL	5.7
1	A	1041	GLN	5.6
1	A	777	SER	5.4
1	A	825	ASN	5.3
1	A	269	ASP	5.3
1	A	1040	PRO	5.2
1	A	489	GLY	5.1
1	A	1092	LEU	5.1
1	A	1042	LEU	4.9
1	A	148	GLN	4.7
1	A	1044	SER	4.6
1	A	896	VAL	4.5
1	A	982	ARG	4.5
1	A	999	GLY	4.4
1	A	837	ASP	4.2
1	A	253	ALA	4.1
1	A	254	LYS	4.0
1	A	528	ALA	3.8
1	A	898	ASN	3.7
1	A	374	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	378	ASP	3.6
1	A	981	GLU	3.6
1	A	1046	GLU	3.6
1	A	821	THR	3.5
1	A	936	CYS	3.5
1	A	822	ALA	3.5
1	A	249	PHE	3.5
1	A	874	ASP	3.5
1	A	757	TYR	3.4
1	A	824	SER	3.4
1	A	217	ASN	3.4
1	A	755	GLU	3.4
1	A	939	THR	3.3
1	A	270	PHE	3.2
1	A	219	CYS	3.2
1	A	321	GLU	3.2
1	A	373	LEU	3.1
1	A	895	THR	3.1
1	A	147	SER	3.0
1	A	376	ASN	3.0
1	A	778	GLN	3.0
1	A	370	ILE	3.0
1	A	772	GLU	3.0
1	A	175	PHE	2.9
1	A	1000	LYS	2.9
1	A	544	ARG	2.9
1	A	937	VAL	2.9
1	A	229	THR	2.9
1	A	250	THR	2.9
1	A	613	ARG	2.8
1	A	1043	THR	2.8
1	A	375	ARG	2.8
1	A	516	ILE	2.7
1	A	246	GLN	2.7
1	A	281	LEU	2.7
1	A	952	ILE	2.7
1	A	716	ILE	2.7
1	A	320	LYS	2.7
1	A	826	GLU	2.6
1	A	1088	LEU	2.6
1	A	894	SER	2.6
1	A	938	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	932	CYS	2.6
1	A	227	SER	2.6
1	A	685	GLY	2.6
1	A	305	VAL	2.5
1	A	756	LYS	2.5
1	A	967	HIS	2.4
1	A	933	ALA	2.4
1	A	998	SER	2.4
1	A	228	THR	2.4
1	A	592	LEU	2.4
1	A	1064	ALA	2.4
1	A	609	GLN	2.4
1	A	1063	ASP	2.4
1	A	682	LEU	2.4
1	A	962	HIS	2.3
1	A	615	GLU	2.3
1	A	429	LEU	2.3
1	A	752	LEU	2.3
1	A	146	GLU	2.3
1	A	226	ARG	2.3
1	A	359	ARG	2.3
1	A	739	ILE	2.3
1	A	809	LYS	2.2
1	A	742	LEU	2.2
1	A	935	TYR	2.2
1	A	899	THR	2.2
1	A	398	ARG	2.1
1	A	612	ALA	2.1
1	A	382	PHE	2.1
1	A	836	ASP	2.1
1	A	464	VAL	2.1
1	A	431	LEU	2.1
1	A	1060	ASN	2.1
1	A	986	VAL	2.1
1	A	379	LEU	2.1
1	A	811	LEU	2.0
1	A	222	ILE	2.0
1	A	720	TYR	2.0
1	A	732	PHE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	STU	A	3001	35/35	0.78	0.29	2.13	74,78,84,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.