



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:45 am GMT

PDB ID : 1E8X  
Title : STRUCTURAL INSIGHTS INTO PHOSHOINOSITIDE 3-KINASE ENZY-  
MATIC MECHANISM AND SIGNALLING  
Authors : Walker, E.H.; Perisic, O.; Ried, C.; Stephens, L.; Williams, R.L.  
Deposited on : 2000-10-03  
Resolution : 2.20 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

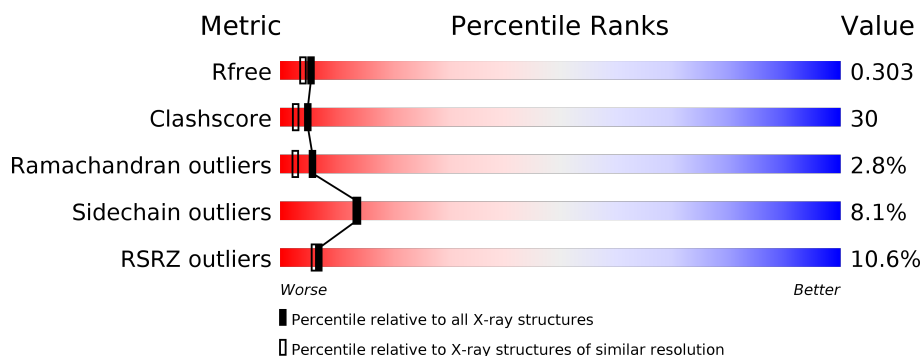
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	961	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7098 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.

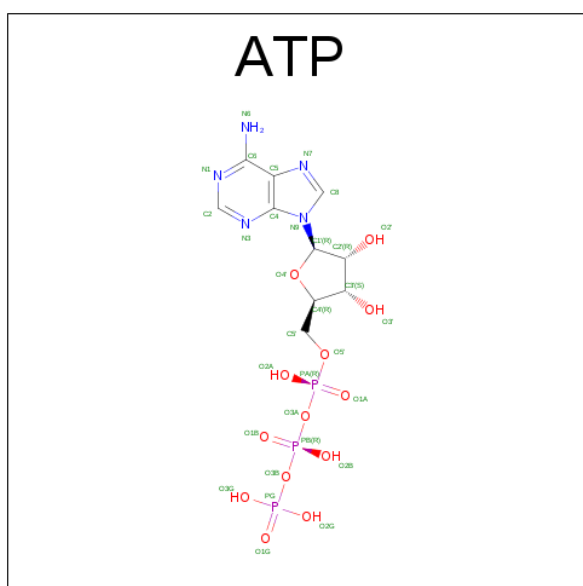
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	841	6805	4375	1154	1240	36	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ALA	-	EXPRESSION TAG	UNP O02697
A	143	ALA	-	EXPRESSION TAG	UNP O02697
A	505	ALA	ARG	CONFLICT	UNP O02697

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	5	13	3	0	0

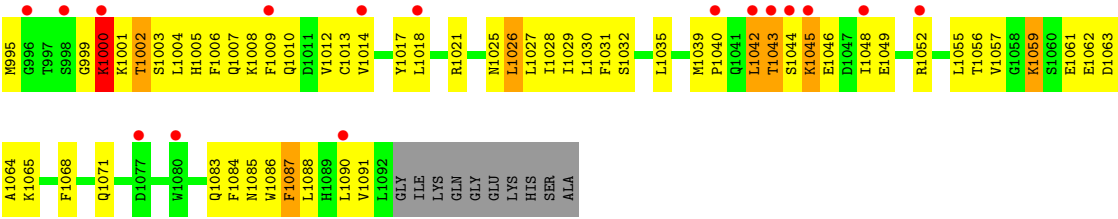
- Molecule 3 is LUTETIUM (III) ION (three-letter code: LU) (formula: Lu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total 9	Lu 9	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	253	Total 253	O 253	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.29Å 67.56Å 106.95Å 90.00° 95.93° 90.00°	Depositor
Resolution (Å)	100.00 – 2.20 106.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.4 (100.00-2.20) 95.5 (106.38-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.255 , 0.306 0.252 , 0.303	Depositor DCC
$R_{free}$ test set	2776 reflections (5.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 69.2	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	0.94	EDS
Total number of atoms	7098	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: LU, ATP

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	0.71	0/6946	0.78	3/9396 (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	641	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	A	484	MET	N-CA-C	5.57	126.03	111.00
1	A	845	LEU	CA-CB-CG	5.04	126.90	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	6805	0	6872	414	0
2	A	31	0	12	1	0
3	A	9	0	0	0	0
4	A	253	0	0	23	1
All	All	7098	0	6884	414	1

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 30.



All (414) 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:641:ARG:HD3	1:A:670:GLU:OE2	1.56	1.04
1:A:629:GLN:HG2	1:A:1029:ILE:HG21	1.45	0.99
1:A:662:GLN:HE22	1:A:850:ILE:HD11	1.31	0.95
1:A:561:THR:HB	1:A:1025:ASN:HD21	1.36	0.89
1:A:583:LEU:O	1:A:583:LEU:HD23	1.76	0.85
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.57	0.84
1:A:246:GLN:HG3	1:A:268:ARG:HH22	1.40	0.84
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.44	0.83
1:A:561:THR:O	1:A:563:PRO:HD3	1.79	0.83
1:A:214:LYS:NZ	1:A:300:GLY:HA2	1.94	0.83
1:A:380:THR:HG23	1:A:435:CYS:SG	2.19	0.82
1:A:1029:ILE:HD12	1:A:1030:LEU:N	1.94	0.82
1:A:158:ILE:HD11	1:A:721:LEU:HD12	1.62	0.82
1:A:1059:LYS:HE3	1:A:1063:ASP:HB3	1.60	0.81
1:A:481:VAL:HG12	4:A:2084:HOH:O	1.79	0.81
1:A:370:ILE:HD13	1:A:371:PRO:N	1.94	0.81
1:A:200:PRO:HG3	1:A:282:VAL:HG23	1.61	0.81
1:A:145:GLU:HA	1:A:148:LEU:HD12	1.64	0.80
1:A:893:GLN:HB3	1:A:898:ASN:OD1	1.81	0.79
1:A:583:LEU:HD12	1:A:610:LEU:HD22	1.64	0.79
1:A:1029:ILE:HD12	1:A:1030:LEU:H	1.47	0.79
1:A:246:GLN:HA	1:A:268:ARG:HH12	1.49	0.78
1:A:143:ALA:HB3	1:A:148:LEU:HD21	1.65	0.78
1:A:693:HIS:CD2	1:A:789:PRO:HG3	2.19	0.78
1:A:370:ILE:HD13	1:A:371:PRO:CD	2.14	0.77
1:A:778:ASN:HD22	1:A:778:ASN:N	1.82	0.77
1:A:739:ILE:O	1:A:743:GLN:HG3	1.86	0.76
1:A:807:LYS:HE3	1:A:807:LYS:H	1.50	0.76
1:A:1087:PHE:O	1:A:1091:VAL:HG23	1.87	0.75
1:A:1059:LYS:HG2	1:A:1063:ASP:HB2	1.69	0.74
1:A:851:MET:HE1	1:A:938:ALA:HA	1.69	0.74
1:A:207:LEU:HD11	1:A:288:LYS:HD2	1.69	0.74
1:A:629:GLN:HG2	1:A:1029:ILE:CG2	2.16	0.74
1:A:891:ILE:HG22	1:A:906:VAL:HG12	1.68	0.74
1:A:555:LEU:HD23	1:A:556:GLU:HG3	1.70	0.73
1:A:237:ALA:HA	1:A:287:ILE:HD11	1.70	0.73
1:A:182:THR:HB	1:A:183:PRO:HD3	1.70	0.73
1:A:302:GLU:CD	1:A:304:HIS:HE2	1.91	0.73
1:A:887:THR:HG22	1:A:889:ALA:H	1.53	0.73
1:A:402:LYS:HB3	1:A:403:PRO:HD2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:GLN:HE22	1:A:850:ILE:CD1	2.02	0.72
1:A:757:TYR:HA	1:A:809:LYS:NZ	2.05	0.72
1:A:359:ARG:HG3	1:A:360:LYS:N	2.04	0.72
1:A:662:GLN:NE2	1:A:850:ILE:HD11	2.03	0.72
1:A:287:ILE:HG23	4:A:2035:HOH:O	1.89	0.72
1:A:555:LEU:HD23	1:A:556:GLU:N	2.04	0.72
1:A:853:SER:O	1:A:857:THR:HG23	1.90	0.71
1:A:1055:LEU:O	1:A:1056:THR:HG22	1.90	0.71
1:A:184:ARG:NH1	1:A:722:ARG:HD2	2.06	0.71
1:A:312:ASP:OD2	1:A:314:ALA:HB3	1.90	0.71
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.72	0.71
1:A:287:ILE:HD12	1:A:288:LYS:N	2.06	0.71
1:A:807:LYS:HE3	1:A:807:LYS:N	2.05	0.71
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.07	0.70
1:A:552:ARG:HD3	1:A:581:GLU:HG2	1.73	0.70
1:A:935:TYR:O	1:A:939:THR:HG22	1.92	0.70
1:A:641:ARG:HD3	1:A:670:GLU:CD	2.13	0.69
1:A:460:LEU:HD23	1:A:487:LEU:HD11	1.73	0.69
1:A:1017:TYR:O	1:A:1021:ARG:HG3	1.94	0.68
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.74	0.68
1:A:1045:LYS:H	1:A:1048:ILE:HD12	1.59	0.68
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.75	0.68
1:A:158:ILE:HD12	1:A:717:LEU:HB3	1.73	0.67
1:A:187:GLU:OE1	1:A:687:ARG:HG2	1.94	0.67
1:A:947:ARG:HH11	1:A:947:ARG:HB3	1.58	0.67
1:A:515:SER:HB2	4:A:2084:HOH:O	1.93	0.67
1:A:1014:VAL:HG12	1:A:1018:LEU:HD23	1.76	0.67
1:A:158:ILE:CD1	1:A:721:LEU:HD12	2.26	0.66
1:A:150:PHE:O	1:A:153:GLN:HG2	1.95	0.66
1:A:1061:GLU:HG3	1:A:1062:GLU:OE2	1.96	0.65
1:A:896:VAL:HG12	1:A:897:GLY:H	1.61	0.65
1:A:246:GLN:HA	1:A:268:ARG:NH1	2.11	0.65
1:A:662:GLN:NE2	1:A:850:ILE:CD1	2.59	0.65
1:A:379:LEU:HD22	1:A:435:CYS:SG	2.37	0.64
1:A:235:VAL:HG22	1:A:239:ASP:OD2	1.97	0.64
1:A:245:LEU:HD21	1:A:272:LEU:HG	1.79	0.63
1:A:583:LEU:HB2	4:A:2111:HOH:O	1.96	0.63
1:A:379:LEU:HD22	1:A:380:THR:HG22	1.80	0.63
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.34	0.63
1:A:552:ARG:O	1:A:555:LEU:HD22	1.98	0.62
1:A:211:LEU:HD21	1:A:298:LYS:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:TRP:O	1:A:579:ARG:HG3	1.99	0.62
1:A:625:GLY:O	1:A:629:GLN:HG3	1.99	0.62
1:A:162:VAL:CG1	1:A:714:ALA:HB1	2.30	0.62
1:A:675:SER:O	1:A:679:ARG:HG3	1.99	0.62
1:A:276:GLY:HA2	1:A:819:ASP:OD2	1.99	0.61
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.81	0.61
1:A:1084:PHE:CE2	1:A:1088:LEU:HD11	2.36	0.61
1:A:989:PRO:HA	1:A:992:LEU:HD12	1.82	0.61
1:A:151:GLN:HA	1:A:154:LEU:HD12	1.81	0.61
1:A:929:VAL:HG22	1:A:995:MET:HE3	1.83	0.61
1:A:157:LEU:HA	4:A:2003:HOH:O	2.01	0.61
1:A:555:LEU:CD2	1:A:556:GLU:HG3	2.30	0.61
1:A:1049:GLU:HG3	1:A:1052:ARG:NH2	2.15	0.60
1:A:221:PHE:HD2	1:A:234:LYS:HG2	1.65	0.60
1:A:213:LYS:HD3	1:A:214:LYS:N	2.17	0.60
1:A:158:ILE:HD13	1:A:717:LEU:HD13	1.82	0.60
1:A:1006:PHE:O	1:A:1010:GLN:HG3	2.01	0.60
1:A:602:GLU:O	1:A:605:ALA:HB3	2.01	0.60
1:A:955:SER:C	1:A:957:THR:H	2.05	0.59
1:A:549:ASN:H	1:A:549:ASN:ND2	2.01	0.59
1:A:380:THR:O	1:A:435:CYS:HB3	2.02	0.59
1:A:629:GLN:CG	1:A:1029:ILE:HG21	2.28	0.59
1:A:753:SER:O	1:A:809:LYS:HE3	2.03	0.59
1:A:652:GLU:HA	4:A:2130:HOH:O	2.03	0.59
1:A:851:MET:HE1	1:A:938:ALA:CA	2.32	0.59
1:A:772:GLU:HG2	1:A:798:ILE:HD13	1.85	0.59
1:A:143:ALA:CB	1:A:148:LEU:HD21	2.33	0.58
1:A:370:ILE:HD13	1:A:371:PRO:HD2	1.84	0.58
1:A:497:PHE:HB3	4:A:2242:HOH:O	2.02	0.58
1:A:804:MET:CE	1:A:810:PRO:HB2	2.32	0.58
1:A:525:HIS:HB3	1:A:526:PRO:HD3	1.86	0.58
1:A:221:PHE:CD2	1:A:234:LYS:HG2	2.39	0.58
1:A:219:CYS:HA	1:A:236:SER:HA	1.86	0.58
1:A:370:ILE:HD12	1:A:372:VAL:O	2.03	0.58
1:A:144:SER:HB2	1:A:147:THR:OG1	2.04	0.57
1:A:899:THR:HA	1:A:1087:PHE:CZ	2.38	0.57
1:A:624:VAL:O	1:A:628:MET:HG2	2.04	0.57
1:A:470:ASP:OD1	1:A:472:ARG:N	2.37	0.57
1:A:187:GLU:OE2	1:A:687:ARG:HD3	2.04	0.57
1:A:808:LYS:HD2	1:A:835:GLY:HA3	1.85	0.57
1:A:851:MET:HE1	1:A:938:ALA:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:SER:O	1:A:860:LEU:HD23	2.05	0.57
1:A:271:VAL:HG12	1:A:308:ASP:O	2.04	0.57
1:A:947:ARG:NH1	1:A:947:ARG:HB3	2.19	0.57
1:A:1062:GLU:H	1:A:1062:GLU:CD	2.09	0.57
1:A:162:VAL:HG23	1:A:177:ARG:NH1	2.19	0.56
1:A:302:GLU:HB2	1:A:304:HIS:CD2	2.40	0.56
1:A:240:THR:CG2	1:A:242:GLY:H	2.17	0.56
1:A:947:ARG:HD3	1:A:962:HIS:ND1	2.20	0.56
1:A:1044:SER:O	1:A:1046:GLU:N	2.39	0.56
1:A:799:GLU:H	1:A:799:GLU:CD	2.08	0.56
1:A:393:VAL:O	1:A:393:VAL:HG23	2.05	0.56
1:A:757:TYR:HA	1:A:809:LYS:HZ1	1.71	0.56
1:A:1045:LYS:O	1:A:1049:GLU:HB2	2.06	0.55
1:A:1056:THR:HG23	1:A:1056:THR:O	2.07	0.55
1:A:955:SER:OG	1:A:957:THR:HG22	2.06	0.55
1:A:683:LYS:HD2	4:A:2144:HOH:O	2.06	0.55
1:A:804:MET:HE3	1:A:810:PRO:HB2	1.86	0.55
1:A:273:ARG:NH1	1:A:308:ASP:OD2	2.39	0.55
1:A:232:THR:C	1:A:233:ILE:HD12	2.26	0.55
1:A:548:PRO:HB2	1:A:552:ARG:CB	2.36	0.55
1:A:421:LYS:NZ	1:A:526:PRO:HB3	2.22	0.55
1:A:163:THR:HG22	1:A:177:ARG:HH22	1.72	0.55
1:A:290:PHE:O	1:A:294:ARG:HG3	2.07	0.55
1:A:622:LEU:HD11	4:A:2123:HOH:O	2.05	0.55
1:A:293:VAL:O	1:A:297:LEU:HG	2.08	0.54
1:A:852:GLU:HG2	4:A:2203:HOH:O	2.06	0.54
1:A:905:GLU:HA	1:A:993:PHE:CE1	2.43	0.54
1:A:193:PRO:HB2	1:A:313:PRO:HB3	1.87	0.54
1:A:214:LYS:HG2	1:A:214:LYS:O	2.07	0.54
1:A:299:ASN:O	1:A:301:GLU:HG3	2.07	0.54
1:A:767:LEU:HD22	1:A:771:LEU:HD11	1.88	0.54
1:A:804:MET:HE2	1:A:831:ILE:HG12	1.90	0.54
1:A:143:ALA:O	1:A:148:LEU:HD11	2.07	0.54
1:A:1044:SER:C	1:A:1046:GLU:H	2.10	0.54
1:A:222:ILE:O	1:A:222:ILE:HG13	2.08	0.54
1:A:905:GLU:HB3	1:A:909:HIS:CE1	2.43	0.54
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.08	0.54
1:A:552:ARG:O	1:A:555:LEU:HB3	2.07	0.54
1:A:738:VAL:HG22	1:A:780:PRO:HD2	1.90	0.54
1:A:757:TYR:HA	1:A:809:LYS:HZ3	1.73	0.54
1:A:750:LYS:NZ	1:A:834:HIS:HD2	2.05	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:LYS:HG2	1:A:1000:LYS:O	2.07	0.53
1:A:1026:LEU:O	1:A:1029:ILE:HD12	2.08	0.53
1:A:899:THR:HG22	1:A:1087:PHE:HZ	1.73	0.53
1:A:163:THR:HG22	1:A:177:ARG:NH2	2.23	0.53
1:A:552:ARG:HH21	1:A:578:PHE:HA	1.74	0.53
1:A:171:ASP:O	1:A:175:PHE:CB	2.57	0.53
1:A:887:THR:HG22	1:A:889:ALA:N	2.22	0.53
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.54	0.53
1:A:552:ARG:HE	1:A:578:PHE:HB3	1.72	0.53
1:A:245:LEU:HD21	1:A:272:LEU:CG	2.39	0.53
1:A:725:GLY:O	1:A:729:LEU:HG	2.09	0.53
1:A:791:LEU:HD22	1:A:828:ILE:HD11	1.90	0.53
1:A:905:GLU:HB3	1:A:909:HIS:ND1	2.24	0.53
1:A:188:VAL:HG11	1:A:318:VAL:HG11	1.90	0.53
1:A:889:ALA:HB2	1:A:949:ASN:HB3	1.91	0.53
1:A:995:MET:HE1	1:A:1009:PHE:HB2	1.90	0.52
1:A:167:ASN:O	1:A:168:VAL:HG22	2.08	0.52
1:A:935:TYR:CE2	1:A:961:PHE:HA	2.44	0.52
1:A:220:VAL:N	1:A:235:VAL:O	2.32	0.52
1:A:473:PHE:HD2	1:A:527:ILE:HG22	1.73	0.52
1:A:851:MET:CE	1:A:938:ALA:CB	2.87	0.52
1:A:274:VAL:HG23	1:A:279:GLU:O	2.09	0.52
1:A:899:THR:HA	1:A:1087:PHE:CE2	2.44	0.52
1:A:180:LEU:O	1:A:183:PRO:HD2	2.09	0.52
1:A:474:LEU:HD23	1:A:525:HIS:HA	1.90	0.52
1:A:359:ARG:HG3	1:A:360:LYS:H	1.75	0.52
1:A:891:ILE:HG22	1:A:906:VAL:CG1	2.38	0.52
1:A:240:THR:O	1:A:244:ILE:HG12	2.10	0.51
1:A:379:LEU:CD2	1:A:380:THR:HG22	2.40	0.51
1:A:1026:LEU:O	1:A:1029:ILE:CD1	2.58	0.51
1:A:366:ARG:NH1	1:A:479:GLU:OE2	2.43	0.51
1:A:921:PHE:O	1:A:925:VAL:HG23	2.09	0.51
1:A:240:THR:HG22	1:A:242:GLY:H	1.75	0.51
1:A:584:LYS:HA	1:A:616:VAL:HG21	1.91	0.51
1:A:1071:GLN:HA	1:A:1071:GLN:OE1	2.11	0.51
1:A:764:ILE:O	1:A:768:LYS:HG3	2.11	0.51
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.45	0.51
1:A:528:ALA:O	1:A:529:LEU:HB2	2.09	0.51
1:A:552:ARG:CZ	1:A:581:GLU:HB2	2.40	0.51
1:A:784:ARG:NH1	1:A:789:PRO:O	2.43	0.51
1:A:563:PRO:HB2	1:A:1028:ILE:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ASN:O	1:A:218:ASN:HB2	2.11	0.51
1:A:558:ILE:HG12	1:A:571:ASP:OD2	2.10	0.51
1:A:750:LYS:HZ3	1:A:834:HIS:HD2	1.59	0.51
1:A:777:LEU:C	1:A:778:ASN:HD22	2.14	0.51
1:A:1004:LEU:O	1:A:1007:GLN:HB2	2.11	0.51
1:A:809:LYS:N	1:A:810:PRO:HD3	2.26	0.51
1:A:887:THR:HG21	1:A:950:ASP:HA	1.93	0.50
1:A:497:PHE:HA	1:A:1044:SER:OG	2.11	0.50
1:A:914:LYS:HG2	1:A:956:GLU:HG2	1.92	0.50
1:A:311:PRO:O	1:A:313:PRO:HD3	2.11	0.50
1:A:995:MET:O	1:A:1005:HIS:HB2	2.12	0.50
1:A:561:THR:HB	1:A:1025:ASN:ND2	2.17	0.50
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.47	0.50
1:A:1032:SER:HB3	1:A:1048:ILE:HG21	1.94	0.50
1:A:1085:ASN:HA	1:A:1088:LEU:HD12	1.93	0.50
1:A:552:ARG:HH21	1:A:578:PHE:HD1	1.58	0.50
1:A:778:ASN:N	1:A:778:ASN:ND2	2.52	0.50
1:A:552:ARG:HH21	1:A:578:PHE:CB	2.25	0.50
1:A:559:ILE:HD13	1:A:588:ALA:HB2	1.94	0.50
1:A:617:TRP:O	1:A:620:SER:OG	2.29	0.50
1:A:167:ASN:C	1:A:168:VAL:CG2	2.80	0.49
1:A:357:CYS:O	1:A:421:LYS:HD3	2.12	0.49
1:A:807:LYS:H	1:A:807:LYS:CE	2.22	0.49
1:A:548:PRO:HB2	1:A:552:ARG:HD2	1.94	0.49
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.46	0.49
1:A:1031:PHE:O	1:A:1035:LEU:HG	2.13	0.49
1:A:373:LEU:HD12	1:A:374:PRO:HD2	1.93	0.49
1:A:552:ARG:NE	1:A:578:PHE:HB3	2.28	0.49
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.94	0.49
1:A:1086:TRP:O	1:A:1090:LEU:HG	2.13	0.49
1:A:212:LEU:HA	1:A:215:ILE:HD12	1.94	0.49
1:A:568:THR:HG22	1:A:569:ALA:N	2.28	0.49
1:A:736:VAL:HG21	4:A:2003:HOH:O	2.12	0.49
1:A:363:VAL:HG23	1:A:520:LEU:HD12	1.95	0.49
1:A:631:LEU:HD23	1:A:641:ARG:HG3	1.95	0.49
1:A:226:ARG:HB3	1:A:229:THR:HB	1.94	0.49
1:A:359:ARG:CG	1:A:360:LYS:N	2.74	0.49
1:A:616:VAL:HG23	4:A:2119:HOH:O	2.13	0.49
1:A:246:GLN:HG3	1:A:268:ARG:NH2	2.18	0.48
1:A:470:ASP:HB3	1:A:476:ARG:HH21	1.77	0.48
1:A:927:ARG:HH11	1:A:959:ASN:ND2	2.10	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.78	0.48
1:A:205:LYS:HB3	1:A:206:PRO:HD2	1.95	0.48
1:A:569:ALA:O	1:A:573:GLU:HG3	2.13	0.48
1:A:730:HIS:O	1:A:734:GLN:HG2	2.13	0.48
1:A:824:SER:OG	1:A:826:GLU:HG3	2.13	0.48
1:A:995:MET:CE	1:A:1009:PHE:HB2	2.43	0.48
1:A:991:PHE:O	1:A:995:MET:HG3	2.14	0.48
1:A:1084:PHE:O	1:A:1088:LEU:HG	2.14	0.48
1:A:251:LYS:O	1:A:252:MET:HE3	2.14	0.48
1:A:278:ASP:CG	1:A:784:ARG:HH22	2.17	0.48
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.44	0.48
1:A:548:PRO:HG2	1:A:552:ARG:CZ	2.44	0.48
1:A:896:VAL:HG13	1:A:903:LYS:HE3	1.95	0.48
1:A:1035:LEU:HB3	1:A:1042:LEU:HD12	1.96	0.47
1:A:187:GLU:CD	1:A:687:ARG:HG2	2.33	0.47
1:A:552:ARG:NH2	1:A:578:PHE:CD1	2.81	0.47
1:A:887:THR:CG2	1:A:950:ASP:HA	2.44	0.47
1:A:602:GLU:H	1:A:602:GLU:CD	2.18	0.47
1:A:174:GLU:HG3	4:A:2015:HOH:O	2.15	0.47
1:A:907:LEU:HG	1:A:994:VAL:HG21	1.95	0.47
1:A:201:TRP:CD1	1:A:291:GLN:HG3	2.50	0.47
1:A:266:ASN:HD21	1:A:269:ASP:HA	1.80	0.47
1:A:614:ARG:HB3	1:A:618:ASP:OD1	2.15	0.47
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.97	0.47
1:A:472:ARG:O	1:A:473:PHE:HB2	2.14	0.47
1:A:562:ASP:HB3	1:A:565:ASN:HB2	1.95	0.47
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.96	0.47
1:A:235:VAL:HG21	1:A:244:ILE:CD1	2.45	0.46
1:A:1003:SER:HB2	1:A:1006:PHE:HB3	1.96	0.46
1:A:214:LYS:HZ2	1:A:300:GLY:HA2	1.77	0.46
1:A:555:LEU:O	1:A:559:ILE:HG13	2.15	0.46
1:A:851:MET:CE	1:A:938:ALA:HB2	2.44	0.46
1:A:1052:ARG:O	1:A:1057:VAL:HG23	2.14	0.46
1:A:425:LYS:HA	1:A:469:ILE:HD12	1.96	0.46
1:A:576:TRP:O	1:A:579:ARG:CG	2.64	0.46
1:A:1061:GLU:HG3	1:A:1062:GLU:CD	2.36	0.46
1:A:552:ARG:HE	1:A:578:PHE:CB	2.28	0.46
1:A:215:ILE:C	1:A:217:ASN:H	2.19	0.46
1:A:568:THR:H	1:A:571:ASP:HB2	1.79	0.46
1:A:574:LEU:HD23	1:A:578:PHE:HD2	1.79	0.46
1:A:574:LEU:HD23	1:A:578:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:HIS:HD2	4:A:2200:HOH:O	1.99	0.46
1:A:631:LEU:CD2	1:A:641:ARG:HG3	2.45	0.46
1:A:707:ARG:NE	1:A:710:GLN:OE1	2.49	0.46
1:A:743:GLN:HE22	1:A:872:THR:CB	2.29	0.46
1:A:1035:LEU:HA	1:A:1039:MET:HG3	1.98	0.45
1:A:1043:THR:HG22	1:A:1046:GLU:HG3	1.98	0.45
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.81	0.45
1:A:224:ILE:CG2	1:A:307:LEU:HD13	2.46	0.45
1:A:738:VAL:HG12	1:A:742:LEU:HD12	1.98	0.45
1:A:767:LEU:HD22	1:A:771:LEU:CD1	2.47	0.45
1:A:568:THR:HB	1:A:571:ASP:OD1	2.16	0.45
1:A:583:LEU:HD12	1:A:610:LEU:CD2	2.39	0.45
1:A:211:LEU:O	1:A:215:ILE:HG13	2.17	0.45
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.44	0.45
1:A:194:LYS:HG2	1:A:313:PRO:HG2	1.99	0.45
1:A:308:ASP:N	1:A:308:ASP:OD1	2.49	0.45
1:A:548:PRO:HG2	1:A:552:ARG:NE	2.32	0.45
1:A:659:TYR:HB2	4:A:2134:HOH:O	2.16	0.45
1:A:843:LEU:O	1:A:847:ILE:HD13	2.17	0.45
1:A:154:LEU:O	1:A:158:ILE:HG12	2.16	0.44
1:A:470:ASP:OD1	1:A:470:ASP:C	2.56	0.44
1:A:548:PRO:HB2	1:A:552:ARG:HB3	1.97	0.44
1:A:548:PRO:HD2	1:A:552:ARG:NH1	2.32	0.44
1:A:552:ARG:NH2	1:A:578:PHE:HD1	2.14	0.44
1:A:656:VAL:HA	4:A:2134:HOH:O	2.17	0.44
1:A:583:LEU:C	1:A:585:ASP:H	2.21	0.44
1:A:806:SER:HB3	1:A:810:PRO:CD	2.47	0.44
1:A:281:LEU:HA	1:A:290:PHE:CE2	2.52	0.44
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.86	0.44
1:A:233:ILE:N	1:A:233:ILE:HD12	2.33	0.44
1:A:196:TYR:OH	1:A:724:CYS:O	2.28	0.44
1:A:912:LYS:HG2	1:A:921:PHE:CE1	2.52	0.44
1:A:625:GLY:HA2	1:A:1026:LEU:HD23	1.98	0.44
1:A:151:GLN:OE1	1:A:722:ARG:NH2	2.50	0.44
1:A:559:ILE:O	1:A:559:ILE:HG22	2.18	0.44
1:A:558:ILE:C	1:A:560:ALA:H	2.20	0.44
1:A:755:GLU:HB2	4:A:2172:HOH:O	2.16	0.44
1:A:386:ASN:HB2	1:A:430:ASN:HB3	1.99	0.44
1:A:639:ASN:O	1:A:643:ILE:HG23	2.17	0.44
1:A:804:MET:CE	1:A:831:ILE:HD13	2.48	0.44
1:A:549:ASN:H	1:A:549:ASN:HD22	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLN:NE2	1:A:155:ASN:OD1	2.51	0.43
1:A:476:ARG:O	1:A:520:LEU:HD23	2.17	0.43
1:A:552:ARG:HH21	1:A:578:PHE:CA	2.31	0.43
1:A:646:GLN:HB3	4:A:2127:HOH:O	2.17	0.43
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.18	0.43
1:A:1048:ILE:HG22	1:A:1048:ILE:O	2.18	0.43
1:A:379:LEU:HD13	1:A:435:CYS:SG	2.59	0.43
1:A:1021:ARG:HH21	1:A:1056:THR:HG23	1.84	0.43
1:A:196:TYR:OH	1:A:728:MET:HE2	2.19	0.43
1:A:1008:LYS:O	1:A:1012:VAL:HG23	2.18	0.43
1:A:1088:LEU:O	1:A:1091:VAL:HB	2.19	0.43
1:A:180:LEU:C	1:A:183:PRO:HD2	2.39	0.43
1:A:421:LYS:CE	1:A:526:PRO:HB3	2.48	0.43
1:A:586:PRO:O	1:A:588:ALA:N	2.52	0.43
1:A:884:ASP:O	1:A:884:ASP:OD1	2.37	0.43
1:A:370:ILE:HD13	1:A:370:ILE:C	2.39	0.43
1:A:576:TRP:O	1:A:579:ARG:CD	2.67	0.43
1:A:640:VAL:O	1:A:643:ILE:HG12	2.18	0.43
1:A:266:ASN:ND2	1:A:269:ASP:HA	2.34	0.43
1:A:302:GLU:HB2	1:A:304:HIS:NE2	2.34	0.43
1:A:697:TRP:CH2	1:A:739:ILE:HD13	2.54	0.43
1:A:158:ILE:CD1	1:A:721:LEU:CD1	2.96	0.42
1:A:804:MET:HE1	1:A:810:PRO:HB2	2.00	0.42
1:A:732:PHE:O	1:A:736:VAL:HG23	2.18	0.42
1:A:925:VAL:O	1:A:929:VAL:HG23	2.19	0.42
1:A:167:ASN:C	1:A:168:VAL:HG22	2.39	0.42
1:A:182:THR:CB	1:A:183:PRO:HD3	2.45	0.42
1:A:614:ARG:HD3	1:A:643:ILE:HG21	1.99	0.42
1:A:939:THR:OG1	1:A:945:GLY:HA2	2.19	0.42
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.18	0.42
1:A:1030:LEU:HD23	1:A:1030:LEU:HA	1.78	0.42
1:A:1059:LYS:HE3	1:A:1063:ASP:CB	2.41	0.42
1:A:225:HIS:O	1:A:306:VAL:HG23	2.18	0.42
1:A:228:THR:O	1:A:228:THR:HG22	2.20	0.42
1:A:479:GLU:HG2	1:A:519:LEU:HD13	2.00	0.42
1:A:839:ARG:HA	1:A:842:MET:HE2	2.01	0.42
1:A:583:LEU:C	1:A:583:LEU:HD23	2.40	0.42
1:A:242:GLY:C	1:A:244:ILE:H	2.23	0.42
1:A:847:ILE:HG22	1:A:848:LEU:N	2.35	0.42
1:A:380:THR:CG2	1:A:435:CYS:SG	3.01	0.42
1:A:548:PRO:HB2	1:A:552:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:ASP:O	1:A:994:VAL:HG23	2.20	0.42
1:A:1001:LYS:O	1:A:1002:THR:C	2.58	0.41
1:A:171:ASP:O	1:A:175:PHE:HB3	2.20	0.41
1:A:388:GLN:NE2	4:A:2059:HOH:O	2.53	0.41
1:A:706:SER:O	1:A:710:GLN:HB3	2.20	0.41
1:A:158:ILE:CD1	1:A:717:LEU:HD13	2.49	0.41
1:A:739:ILE:HG13	1:A:740:ASP:N	2.35	0.41
1:A:767:LEU:O	1:A:771:LEU:HG	2.20	0.41
1:A:1021:ARG:HE	1:A:1056:THR:CG2	2.33	0.41
1:A:476:ARG:HB2	1:A:476:ARG:HE	1.44	0.41
1:A:738:VAL:CG2	1:A:780:PRO:HD2	2.50	0.41
1:A:1087:PHE:O	1:A:1087:PHE:HD1	2.03	0.41
1:A:150:PHE:O	1:A:153:GLN:N	2.53	0.41
1:A:162:VAL:HG23	1:A:177:ARG:HH12	1.82	0.41
1:A:990:ASP:OD1	1:A:990:ASP:N	2.53	0.41
1:A:1035:LEU:HA	1:A:1039:MET:CG	2.51	0.41
1:A:240:THR:C	4:A:2035:HOH:O	2.59	0.41
1:A:150:PHE:O	1:A:152:ARG:N	2.53	0.41
1:A:198:MET:HG2	1:A:311:PRO:HD2	2.02	0.41
1:A:428:LEU:HD23	1:A:467:LEU:HD23	2.02	0.41
1:A:903:LYS:HB2	1:A:906:VAL:CG2	2.50	0.41
1:A:527:ILE:HD11	4:A:2074:HOH:O	2.19	0.41
1:A:684:ARG:NH2	4:A:2130:HOH:O	2.53	0.41
1:A:756:LYS:HA	1:A:756:LYS:HE3	2.02	0.41
1:A:1000:LYS:N	1:A:1000:LYS:HD3	2.36	0.41
1:A:243:THR:HG22	1:A:243:THR:O	2.20	0.41
1:A:892:GLN:OE1	1:A:906:VAL:HG21	2.20	0.41
1:A:1084:PHE:HE2	1:A:1088:LEU:HD11	1.84	0.41
1:A:246:GLN:O	1:A:250:THR:HG23	2.20	0.41
1:A:274:VAL:CG2	1:A:279:GLU:HB3	2.51	0.41
1:A:268:ARG:H	1:A:268:ARG:HD3	1.86	0.41
1:A:170:ASP:C	1:A:170:ASP:OD1	2.60	0.41
1:A:463:TYR:CE2	1:A:501:LYS:HA	2.56	0.41
1:A:553:LYS:HD3	1:A:556:GLU:OE2	2.21	0.40
1:A:791:LEU:HD22	1:A:828:ILE:CD1	2.52	0.40
1:A:833:LYS:HD3	2:A:3000:ATP:O1A	2.22	0.40
1:A:361:PHE:HB2	1:A:420:ILE:HD13	2.04	0.40
1:A:576:TRP:CD2	1:A:579:ARG:HD2	2.56	0.40
1:A:892:GLN:HA	1:A:906:VAL:HG11	2.02	0.40
1:A:951:ASN:HD22	1:A:951:ASN:HA	1.66	0.40
1:A:1061:GLU:O	1:A:1064:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:THR:HA	1:A:1087:PHE:HZ	1.85	0.40
1:A:912:LYS:HA	1:A:921:PHE:CD1	2.56	0.40
1:A:947:ARG:CB	1:A:947:ARG:NH1	2.85	0.40
1:A:802:LYS:HE2	4:A:2186:HOH:O	2.21	0.40
1:A:948:HIS:CD2	1:A:950:ASP:HB2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2055:HOH:O	4:A:2055:HOH:O[2_655]	2.09	0.11

## 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	825/961 (86%)	722 (88%)	80 (10%)	23 (3%)	6 3

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	776	ASN
1	A	906	VAL
1	A	358	ASP
1	A	375	ARG
1	A	528	ALA
1	A	561	THR
1	A	900	GLY
1	A	917	ILE
1	A	1002	THR
1	A	999	GLY
1	A	1000	LYS

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Mol	Chain	Res	Type
1	A	1045	LYS
1	A	1059	LYS
1	A	151	GLN
1	A	378	ASP
1	A	559	ILE
1	A	526	PRO
1	A	753	SER
1	A	895	THR
1	A	918	GLU
1	A	548	PRO
1	A	896	VAL
1	A	1040	PRO

### 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	756/857 (88%)	695 (92%)	61 (8%)	14	13

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

Mol	Chain	Res	Type
1	A	145	GLU
1	A	147	THR
1	A	168	VAL
1	A	173	LEU
1	A	187	GLU
1	A	213	LYS
1	A	217	ASN
1	A	221	PHE
1	A	230	SER
1	A	235	VAL
1	A	238	ASP
1	A	240	THR
1	A	252	MET
1	A	268	ARG

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Mol	Chain	Res	Type
1	A	282	VAL
1	A	302	GLU
1	A	308	ASP
1	A	370	ILE
1	A	379	LEU
1	A	380	THR
1	A	381	VAL
1	A	404	PHE
1	A	410	TRP
1	A	476	ARG
1	A	547	MET
1	A	555	LEU
1	A	575	LEU
1	A	594	SER
1	A	626	LEU
1	A	646	GLN
1	A	647	LYS
1	A	682	LEU
1	A	717	LEU
1	A	726	THR
1	A	749	ILE
1	A	756	LYS
1	A	757	TYR
1	A	767	LEU
1	A	775	GLN
1	A	778	ASN
1	A	791	LEU
1	A	792	LYS
1	A	799	GLU
1	A	807	LYS
1	A	838	LEU
1	A	841	ASP
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	899	THR
1	A	913	GLU
1	A	947	ARG
1	A	957	THR
1	A	960	LEU
1	A	983	VAL
1	A	1000	LYS

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Mol	Chain	Res	Type
1	A	1026	LEU
1	A	1027	LEU
1	A	1042	LEU
1	A	1043	THR
1	A	1087	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	153	GLN
1	A	155	ASN
1	A	169	HIS
1	A	225	HIS
1	A	266	ASN
1	A	392	GLN
1	A	522	ASN
1	A	549	ASN
1	A	730	HIS
1	A	743	GLN
1	A	778	ASN
1	A	834	HIS
1	A	948	HIS
1	A	951	ASN
1	A	959	ASN
1	A	1007	GLN
1	A	1025	ASN
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

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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	ATP	A	3000	-	27,33,33	1.89	5 (18%)	25,52,52	1.19	2 (8%)

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	ATP	A	3000	-	-	0/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	ATP	C8-N7	-2.01	1.30	1.34
2	A	3000	ATP	C2'-C1'	2.14	1.57	1.53
2	A	3000	ATP	C2-N3	2.22	1.35	1.32
2	A	3000	ATP	O4'-C1'	2.33	1.44	1.41
2	A	3000	ATP	PG-O3B	7.58	1.72	1.60

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3000	ATP	C4'-O4'-C1'	2.70	112.64	109.77
2	A	3000	ATP	C4-C5-N7	3.18	112.48	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3000	ATP	1	0

## 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	841/961 (87%)	0.84	89 (10%) 7 6	24, 61, 98, 125	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	777	LEU	7.5
1	A	210	TYR	6.9
1	A	561	THR	6.9
1	A	142	ALA	6.6
1	A	552	ARG	6.4
1	A	526	PRO	6.4
1	A	1043	THR	5.5
1	A	143	ALA	5.0
1	A	895	THR	4.7
1	A	522	ASN	4.6
1	A	1044	SER	4.2
1	A	216	THR	4.1
1	A	214	LYS	4.1
1	A	754	ALA	4.1
1	A	1040	PRO	4.0
1	A	918	GLU	4.0
1	A	270	PHE	4.0
1	A	964	ASP	3.8
1	A	998	SER	3.8
1	A	215	ILE	3.7
1	A	474	LEU	3.7
1	A	617	TRP	3.6
1	A	577	HIS	3.6
1	A	916	PRO	3.6
1	A	996	GLY	3.5
1	A	211	LEU	3.5
1	A	377	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	578	PHE	3.3
1	A	319	ARG	3.3
1	A	168	VAL	3.3
1	A	282	VAL	3.2
1	A	755	GLU	3.2
1	A	181	VAL	3.1
1	A	1000	LYS	3.1
1	A	1048	ILE	3.1
1	A	1042	LEU	3.1
1	A	1080	TRP	3.0
1	A	266	ASN	2.9
1	A	528	ALA	2.8
1	A	374	PRO	2.8
1	A	558	ILE	2.8
1	A	249	PHE	2.8
1	A	993	PHE	2.8
1	A	896	VAL	2.8
1	A	753	SER	2.8
1	A	551	LEU	2.7
1	A	245	LEU	2.7
1	A	241	PRO	2.7
1	A	1009	PHE	2.7
1	A	751	SER	2.6
1	A	271	VAL	2.6
1	A	1052	ARG	2.6
1	A	148	LEU	2.6
1	A	147	THR	2.6
1	A	231	GLN	2.5
1	A	560	ALA	2.5
1	A	759	VAL	2.5
1	A	608	TYR	2.4
1	A	287	ILE	2.4
1	A	548	PRO	2.4
1	A	419	LYS	2.4
1	A	372	VAL	2.4
1	A	917	ILE	2.3
1	A	196	TYR	2.3
1	A	178	ARG	2.3
1	A	175	PHE	2.3
1	A	898	ASN	2.3
1	A	171	ASP	2.3
1	A	473	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1090	LEU	2.2
1	A	180	LEU	2.2
1	A	527	ILE	2.2
1	A	948	HIS	2.2
1	A	757	TYR	2.2
1	A	1077	ASP	2.2
1	A	525	HIS	2.1
1	A	1014	VAL	2.1
1	A	153	GLN	2.1
1	A	825	ASN	2.1
1	A	359	ARG	2.1
1	A	1018	LEU	2.1
1	A	557	ALA	2.1
1	A	547	MET	2.1
1	A	185	MET	2.0
1	A	1045	LYS	2.0
1	A	267	GLU	2.0
1	A	268	ARG	2.0
1	A	189	ALA	2.0
1	A	924	ALA	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(Å <sup>2</sup> )	Q<0.9
2	ATP	A	3000	31/31	0.78	0.23	0.53	66,80,92,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LU	A	3008	1/1	0.97	0.06	-	108,108,108,108	0
3	LU	A	3005	1/1	0.97	0.08	-	77,77,77,77	0
3	LU	A	3006	1/1	0.96	0.07	-	86,86,86,86	0
3	LU	A	3001	1/1	0.89	0.11	-	72,72,72,72	0
3	LU	A	3002	1/1	0.87	0.11	-	70,70,70,70	0
3	LU	A	3007	1/1	0.94	0.07	-	121,121,121,121	0
3	LU	A	3009	1/1	0.78	0.07	-	135,135,135,135	0
3	LU	A	3003	1/1	0.97	0.09	-	76,76,76,76	0
3	LU	A	3004	1/1	0.96	0.09	-	72,72,72,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.