



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:30 AM GMT

PDB ID : 1E8X  
Title : STRUCTURAL INSIGHTS INTO PHOSHOINOSITIDE 3-KINASE ENZY-  
MATIC MECHANISM AND SIGNALLING  
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Deposited on : 2000-10-03  
Resolution : 2.20 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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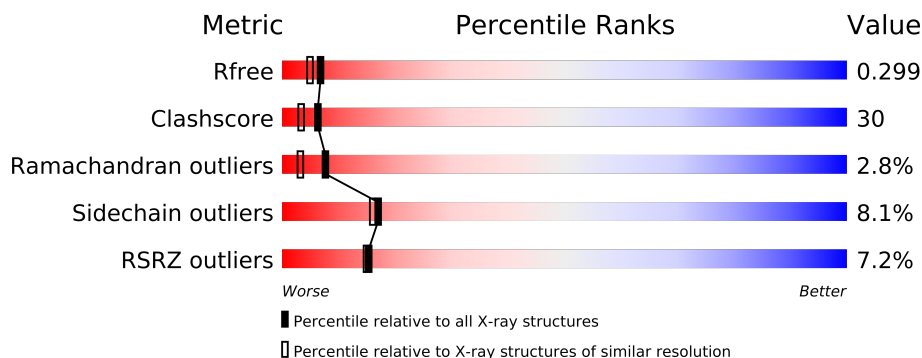
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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. 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	

## 2 Entry composition i

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

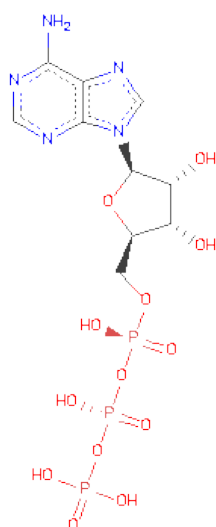
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	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

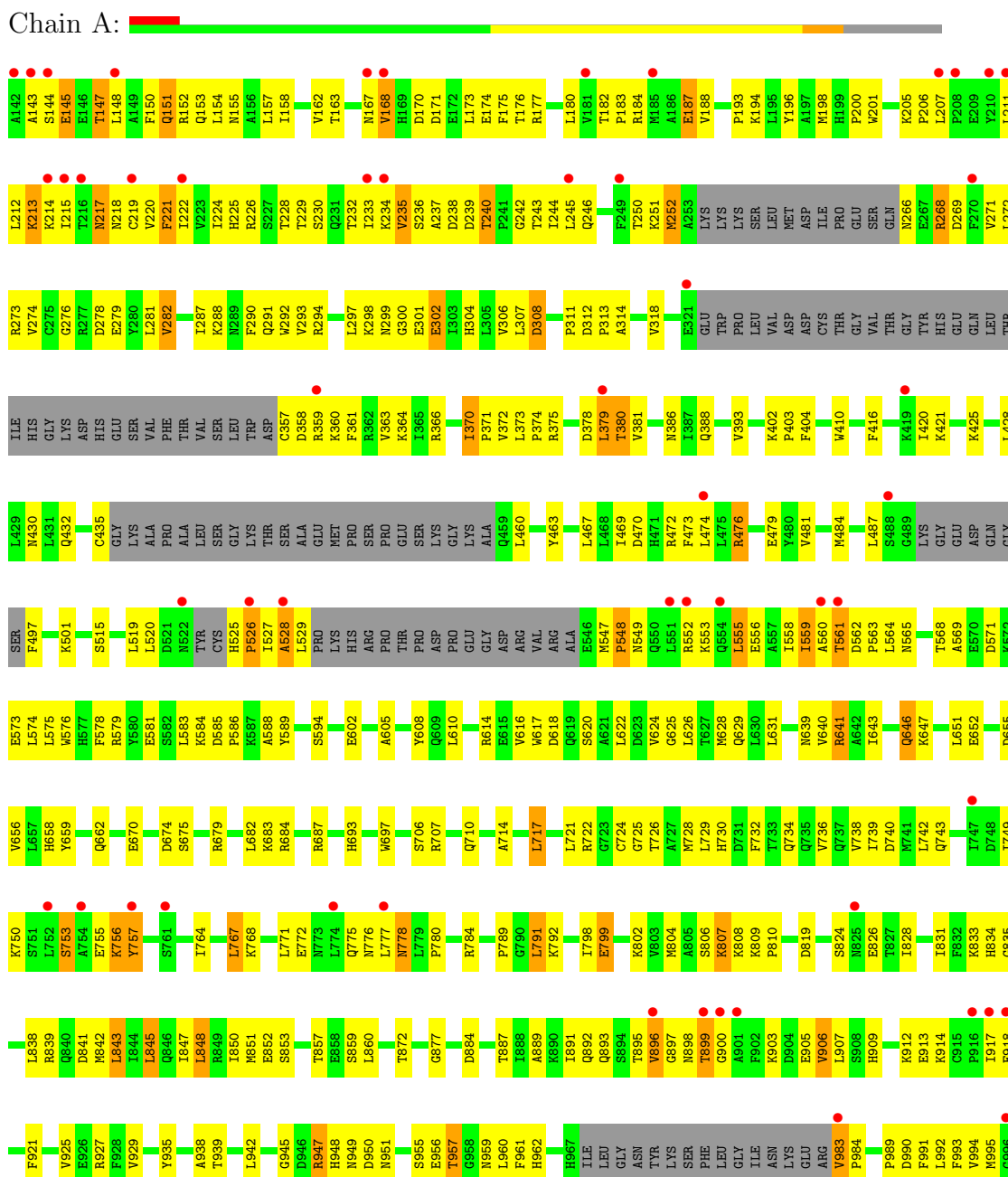
- Molecule 4 is water.

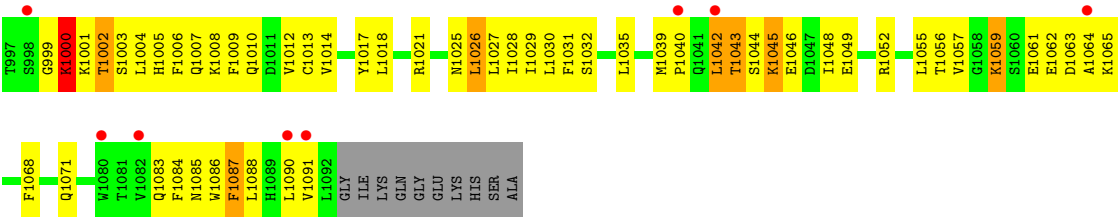
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	253	Total 253	O 253	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUBUNIT





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 0.249 , 0.299	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 , 62.7	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 94074 reflections	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.

## 5 Model quality

### 5.1 Standard geometry

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 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	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



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 30.

All (414) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HD23	1:A:583:LEU:O	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:481:VAL:HG12	4:A:2084:HOH:O	1.79	0.81
1:A:1059:LYS:HE3	1:A:1063:ASP:HB3	1.60	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:402:LYS:HB3	1:A:403:PRO:HD2	1.71	0.73
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: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:1055:LEU:O	1:A:1056:THR:HG22	1.90	0.71
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.72	0.71
1:A:807:LYS:HE3	1:A:807:LYS:N	2.05	0.71
1:A:287:ILE:HD12	1:A:288:LYS:N	2.06	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:576:TRP:O	1:A:579:ARG:HG3	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:211:LEU:HD21	1:A:298:LYS:HG3	1.80	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:555:LEU:CD2	1:A:556:GLU:HG3	2.30	0.61
1:A:157:LEU:HA	4:A:2003:HOH:O	2.01	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:ND2	1:A:549:ASN:H	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:851:MET:HE1	1:A:938:ALA:CA	2.32	0.59
1:A:652:GLU:HA	4:A:2130:HOH:O	2.03	0.59
1:A:772:GLU:HG2	1:A:798:ILE:HD13	1.85	0.59
1:A:370:ILE:HD13	1:A:371:PRO:HD2	1.84	0.58
1:A:143:ALA:CB	1:A:148:LEU:HD21	2.33	0.58
1:A:804:MET:CE	1:A:810:PRO:HB2	2.32	0.58
1:A:497:PHE:HB3	4:A:2242:HOH:O	2.02	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:370:ILE:HD12	1:A:372:VAL:O	2.03	0.58
1:A:219:CYS:HA	1:A:236:SER:HA	1.86	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:851:MET:HE1	1:A:938:ALA:CB	2.34	0.57
1:A:187:GLU:OE2	1:A:687:ARG:HD3	2.04	0.57
1:A:859:SER:O	1:A:860:LEU:HD23	2.05	0.57
1:A:808:LYS:HD2	1:A:835:GLY:HA3	1.85	0.57
1:A:470:ASP:OD1	1:A:472:ARG:N	2.37	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:302:GLU:HB2	1:A:304:HIS:CD2	2.40	0.56
1:A:162:VAL:HG23	1:A:177:ARG:NH1	2.19	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:O	1:A:1056:THR:HG23	2.07	0.55
1:A:955:SER:OG	1:A:957:THR:HG22	2.06	0.55
1:A:804:MET:HE3	1:A:810:PRO:HB2	1.86	0.55
1:A:683:LYS:HD2	4:A:2144:HOH:O	2.06	0.55
1:A:273:ARG:NH1	1:A:308:ASP:OD2	2.39	0.55
1:A:548:PRO:HB2	1:A:552:ARG:CB	2.36	0.55
1:A:232:THR:C	1:A:233:ILE:HD12	2.26	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:622:LEU:HD11	4:A:2123:HOH:O	2.05	0.55
1:A:290:PHE:O	1:A:294:ARG:HG3	2.07	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:905:GLU:HB3	1:A:909:HIS:CE1	2.43	0.54
1:A:222:ILE:O	1:A:222:ILE:HG13	2.08	0.54
1:A:552:ARG:O	1:A:555:LEU:HB3	2.07	0.54
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.08	0.54
1:A:757:TYR:HA	1:A:809:LYS:HZ3	1.73	0.54
1:A:738:VAL:HG22	1:A:780:PRO:HD2	1.90	0.54
1:A:750:LYS:NZ	1:A:834:HIS:HD2	2.05	0.53
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:899:THR:HG22	1:A:1087:PHE:HZ	1.73	0.53
1:A:552:ARG:HH21	1:A:578:PHE:HA	1.74	0.53
1:A:163:THR:HG22	1:A:177:ARG:NH2	2.23	0.53
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.54	0.53
1:A:887:THR:HG22	1:A:889:ALA:N	2.22	0.53
1:A:171:ASP:O	1:A:175:PHE:CB	2.57	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:905:GLU:HB3	1:A:909:HIS:ND1	2.24	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:889:ALA:HB2	1:A:949:ASN:HB3	1.91	0.53
1:A:188:VAL:HG11	1:A:318:VAL:HG11	1.90	0.53
1:A:995:MET:HE1	1:A:1009:PHE:HB2	1.90	0.52
1:A:935:TYR:CE2	1:A:961:PHE:HA	2.44	0.52
1:A:167:ASN:O	1:A:168:VAL:HG22	2.08	0.52
1:A:220:VAL:N	1:A:235:VAL:O	2.32	0.52
1:A:851:MET:CE	1:A:938:ALA:CB	2.87	0.52
1:A:473:PHE:HD2	1:A:527:ILE:HG22	1.73	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:379:LEU:CD2	1:A:380:THR:HG22	2.40	0.51
1:A:240:THR:O	1:A:244:ILE:HG12	2.10	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:784:ARG:NH1	1:A:789:PRO:O	2.43	0.51
1:A:552:ARG:CZ	1:A:581:GLU:HB2	2.40	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:563:PRO:HB2	1:A:1028:ILE:HG21	1.93	0.51
1:A:217:ASN:O	1:A:218:ASN:HB2	2.11	0.51
1:A:777:LEU:C	1:A:778:ASN:HD22	2.14	0.51
1:A:750:LYS:HZ3	1:A:834:HIS:HD2	1.59	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:558:ILE:HG12	1:A:571:ASP:OD2	2.10	0.51
1:A:809:LYS:N	1:A:810:PRO:HD3	2.26	0.51
1:A:1004:LEU:O	1:A:1007:GLN:HB2	2.11	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:807:LYS:H	1:A:807:LYS:CE	2.22	0.49
1:A:357:CYS:O	1:A:421:LYS:HD3	2.12	0.49
1:A:548:PRO:HB2	1:A:552:ARG:HD2	1.94	0.49
1:A:1031:PHE:O	1:A:1035:LEU:HG	2.13	0.49
1:A:552:ARG:NE	1:A:578:PHE:HB3	2.28	0.49
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.46	0.49
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.94	0.49
1:A:373:LEU:HD12	1:A:374:PRO:HD2	1.93	0.49
1:A:212:LEU:HA	1:A:215:ILE:HD12	1.94	0.49
1:A:1086:TRP:O	1:A:1090:LEU:HG	2.13	0.49
1:A:736:VAL:HG21	4:A:2003:HOH:O	2.12	0.49
1:A:568:THR:HG22	1:A:569:ALA:N	2.28	0.49
1:A:631:LEU:HD23	1:A:641:ARG:HG3	1.95	0.49
1:A:363:VAL:HG23	1:A:520:LEU:HD12	1.95	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:226:ARG:HB3	1:A:229:THR:HB	1.94	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
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.78	0.48
1:A:569:ALA:O	1:A:573:GLU:HG3	2.13	0.48
1:A:205:LYS:HB3	1:A:206:PRO:HD2	1.95	0.48
1:A:730:HIS:O	1:A:734:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:278:ASP:CG	1:A:784:ARG:HH22	2.17	0.48
1:A:1084:PHE:O	1:A:1088:LEU:HG	2.14	0.48
1:A:896:VAL:HG13	1:A:903:LYS:HE3	1.95	0.48
1:A:548:PRO:HG2	1:A:552:ARG:CZ	2.44	0.48
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.44	0.48
1:A:251:LYS:O	1:A:252:MET:HE3	2.14	0.48
1:A:1035:LEU:HB3	1:A:1042:LEU:HD12	1.96	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:187:GLU:CD	1:A:687:ARG:HG2	2.33	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:651:LEU:HD22	1:A:655:ASP:HB3	1.96	0.47
1:A:562:ASP:HB3	1:A:565:ASN:HB2	1.95	0.47
1:A:235:VAL:HG21	1:A:244:ILE:CD1	2.45	0.46
1:A:214:LYS:HZ2	1:A:300:GLY:HA2	1.77	0.46
1:A:851:MET:CE	1:A:938:ALA:HB2	2.44	0.46
1:A:555:LEU:O	1:A:559:ILE:HG13	2.15	0.46
1:A:1003:SER:HB2	1:A:1006:PHE:HB3	1.96	0.46
1:A:1052:ARG:O	1:A:1057:VAL:HG23	2.14	0.46
1:A:576:TRP:O	1:A:579:ARG:CG	2.64	0.46
1:A:425:LYS:HA	1:A:469:ILE:HD12	1.96	0.46
1:A:552:ARG:HE	1:A:578:PHE:CB	2.28	0.46
1:A:1061:GLU:HG3	1:A:1062:GLU:CD	2.36	0.46
1:A:215:ILE:C	1:A:217:ASN:H	2.19	0.46
1:A:574:LEU:HD23	1:A:578:PHE:HD2	1.79	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:CD2	2.51	0.46
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:743:GLN:HE22	1:A:872:THR:CB	2.29	0.46
1:A:707:ARG:NE	1:A:710:GLN:OE1	2.49	0.46
1:A:1035:LEU:HA	1:A:1039:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:767:LEU:HD22	1:A:771:LEU:CD1	2.47	0.45
1:A:738:VAL:HG12	1:A:742:LEU:HD12	1.98	0.45
1:A:224:ILE:CG2	1:A:307:LEU:HD13	2.46	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:548:PRO:HG2	1:A:552:ARG:NE	2.32	0.45
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.44	0.45
1:A:308:ASP:N	1:A:308:ASP:OD1	2.49	0.45
1:A:194:LYS:HG2	1:A:313:PRO:HG2	1.99	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:548:PRO:HD2	1:A:552:ARG:NH1	2.32	0.44
1:A:548:PRO:HB2	1:A:552:ARG:HB3	1.97	0.44
1:A:552:ARG:NH2	1:A:578:PHE:HD1	2.14	0.44
1:A:470:ASP:OD1	1:A:470:ASP:C	2.56	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:804:MET:CE	1:A:831:ILE:HD13	2.48	0.44
1:A:639:ASN:O	1:A:643:ILE:HG23	2.17	0.44
1:A:386:ASN:HB2	1:A:430:ASN:HB3	1.99	0.44
1:A:549:ASN:H	1:A:549:ASN:HD22	1.65	0.44
1:A:151:GLN:NE2	1:A:155:ASN:OD1	2.51	0.43
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.18	0.43
1:A:552:ARG:HH21	1:A:578:PHE:CA	2.31	0.43
1:A:476:ARG:O	1:A:520:LEU:HD23	2.17	0.43
1:A:646:GLN:HB3	4:A:2127:HOH:O	2.17	0.43
1:A:1048:ILE:HG22	1:A:1048:ILE:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:1088:LEU:O	1:A:1091:VAL:HB	2.19	0.43
1:A:586:PRO:O	1:A:588:ALA:N	2.52	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:1008:LYS:O	1:A:1012:VAL:HG23	2.18	0.43
1:A:884:ASP:O	1:A:884:ASP:OD1	2.37	0.43
1:A:370:ILE:C	1:A:370:ILE:HD13	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:697:TRP:CH2	1:A:739:ILE:HD13	2.54	0.43
1:A:302:GLU:HB2	1:A:304:HIS:NE2	2.34	0.43
1:A:266:ASN:ND2	1:A:269:ASP:HA	2.34	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:925:VAL:O	1:A:929:VAL:HG23	2.19	0.42
1:A:732:PHE:O	1:A:736:VAL:HG23	2.18	0.42
1:A:182:THR:CB	1:A:183:PRO:HD3	2.45	0.42
1:A:939:THR:OG1	1:A:945:GLY:HA2	2.19	0.42
1:A:167:ASN:C	1:A:168:VAL:HG22	2.39	0.42
1:A:614:ARG:HD3	1:A:643:ILE:HG21	1.99	0.42
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.18	0.42
1:A:1030:LEU:HA	1:A:1030:LEU:HD23	1.78	0.42
1:A:1059:LYS:HE3	1:A:1063:ASP:CB	2.41	0.42
1:A:479:GLU:HG2	1:A:519:LEU:HD13	2.00	0.42
1:A:228:THR:O	1:A:228:THR:HG22	2.20	0.42
1:A:225:HIS:O	1:A:306:VAL:HG23	2.18	0.42
1:A:839:ARG:HA	1:A:842:MET:HE2	2.01	0.42
1:A:583:LEU:HD23	1:A:583:LEU:C	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
1:A:990:ASP:O	1:A:994:VAL:HG23	2.20	0.42
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:171:ASP:O	1:A:175:PHE:HB3	2.20	0.41
1:A:706:SER:O	1:A:710:GLN:HB3	2.20	0.41
1:A:1001:LYS:O	1:A:1002:THR:C	2.58	0.41
1:A:388:GLN:NE2	4:A:2059:HOH:O	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:903:LYS:HB2	1:A:906:VAL:CG2	2.50	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:684:ARG:NH2	4:A:2130:HOH:O	2.53	0.41
1:A:527:ILE:HD11	4:A:2074:HOH:O	2.19	0.41
1:A:756:LYS:HA	1:A:756:LYS:HE3	2.02	0.41
1:A:892:GLN:OE1	1:A:906:VAL:HG21	2.20	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:246:GLN:O	1:A:250:THR:HG23	2.20	0.41
1:A:268:ARG:HD3	1:A:268:ARG:H	1.86	0.41
1:A:1084:PHE:HE2	1:A:1088:LEU:HD11	1.84	0.41
1:A:274:VAL:CG2	1:A:279:GLU:HB3	2.51	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:892:GLN:HA	1:A:906:VAL:HG11	2.02	0.40
1:A:576:TRP:CD2	1:A:579:ARG:HD2	2.56	0.40
1:A:951:ASN:HD22	1:A:951:ASN:HA	1.66	0.40
1:A:361:PHE:HB2	1:A:420:ILE:HD13	2.04	0.40
1:A:899:THR:HA	1:A:1087:PHE:HZ	1.85	0.40
1:A:947:ARG:CB	1:A:947:ARG:NH1	2.85	0.40
1:A:1061:GLU:O	1:A:1064:ALA:HB3	2.21	0.40
1:A:912:LYS:HA	1:A:921:PHE:CD1	2.56	0.40
1:A:948:HIS:CD2	1:A:950:ASP:HB2	2.57	0.40
1:A:802:LYS:HE2	4:A:2186:HOH:O	2.21	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	Distance(Å)	Clash(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%)	<b>8</b> <b>3</b>

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
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%)	17	16

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 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 ⓘ

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	-	33,33,33	2.05	6 (18%)	52,52,52	1.39	4 (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	ATP	A	3000	-	-	0/22/38/38	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	ATP	PG-O3B	6.98	1.72	1.60
2	A	3000	ATP	PB-O3B	6.35	1.71	1.59
2	A	3000	ATP	C2'-C1'	2.53	1.57	1.53
2	A	3000	ATP	PA-O3A	2.05	1.63	1.59
2	A	3000	ATP	O4'-C1'	2.04	1.44	1.41
2	A	3000	ATP	PG-O2G	-2.04	1.47	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3000	ATP	C3'-C2'-C1'	4.89	108.56	100.91
2	A	3000	ATP	C4-C5-N7	3.45	112.48	109.52
2	A	3000	ATP	C8-N9-C4	-3.39	104.31	106.90
2	A	3000	ATP	C4'-O4'-C1'	2.66	112.64	109.75

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	841/961 (87%)	0.58	61 (7%) 15 14	24, 61, 98, 125	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	ALA	9.0
1	A	561	THR	7.2
1	A	560	ALA	7.0
1	A	143	ALA	7.0
1	A	210	TYR	5.6
1	A	552	ARG	4.9
1	A	901	ALA	4.6
1	A	270	PHE	3.9
1	A	211	LEU	3.8
1	A	996	GLY	3.6
1	A	917	ILE	3.4
1	A	554	GLN	3.4
1	A	168	VAL	3.4
1	A	1090	LEU	3.3
1	A	998	SER	3.3
1	A	419	LYS	3.2
1	A	757	TYR	3.1
1	A	896	VAL	3.0
1	A	916	PRO	2.9
1	A	321	GLU	2.9
1	A	167	ASN	2.9
1	A	526	PRO	2.9
1	A	777	LEU	2.8
1	A	1080	TRP	2.8
1	A	214	LYS	2.7
1	A	148	LEU	2.7
1	A	900	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	207	LEU	2.7
1	A	233	ILE	2.7
1	A	551	LEU	2.7
1	A	1091	VAL	2.6
1	A	234	LYS	2.6
1	A	144	SER	2.5
1	A	215	ILE	2.5
1	A	219	CYS	2.5
1	A	522	ASN	2.4
1	A	474	LEU	2.4
1	A	216	THR	2.4
1	A	222	ILE	2.4
1	A	899	THR	2.3
1	A	747	ILE	2.3
1	A	359	ARG	2.3
1	A	245	LEU	2.3
1	A	488	SER	2.3
1	A	528	ALA	2.3
1	A	1082	VAL	2.3
1	A	761	SER	2.3
1	A	1042	LEU	2.2
1	A	754	ALA	2.2
1	A	1064	ALA	2.2
1	A	918	GLU	2.1
1	A	249	PHE	2.1
1	A	825	ASN	2.1
1	A	181	VAL	2.1
1	A	185	MET	2.1
1	A	752	LEU	2.1
1	A	774	LEU	2.1
1	A	379	LEU	2.1
1	A	1040	PRO	2.1
1	A	208	PRO	2.0
1	A	983	VAL	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(Å <sup>2</sup> )	Q<0.9
2	ATP	A	3000	31/31	0.16	-0.01	66,80,92,93	0
3	LU	A	3001	1/1	0.12	-0.82	72,72,72,72	0
3	LU	A	3005	1/1	0.11	-1.17	77,77,77,77	0
3	LU	A	3008	1/1	0.10	-3.30	108,108,108,108	0
3	LU	A	3006	1/1	0.07	-3.64	86,86,86,86	0
3	LU	A	3009	1/1	0.08	-5.78	135,135,135,135	0
3	LU	A	3007	1/1	0.07	-6.43	121,121,121,121	0
3	LU	A	3002	1/1	0.07	-65.00	70,70,70,70	0
3	LU	A	3003	1/1	0.10	-	76,76,76,76	0
3	LU	A	3004	1/1	0.07	-	72,72,72,72	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.