



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:47 PM UTC

PDB ID : 1E8X / pdb_00001e8x
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

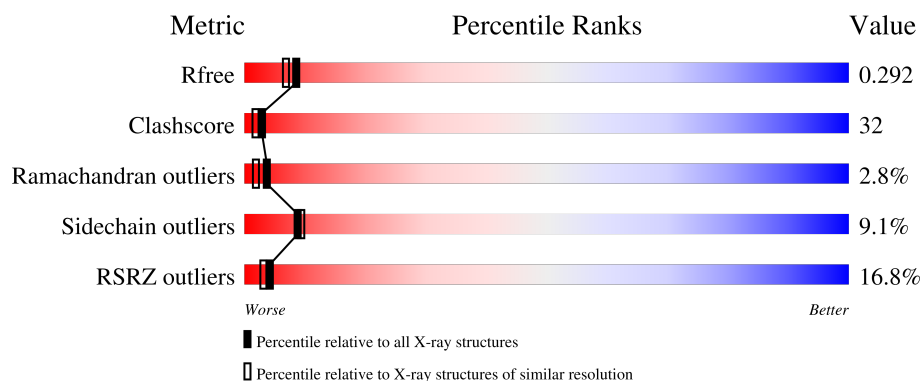
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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.

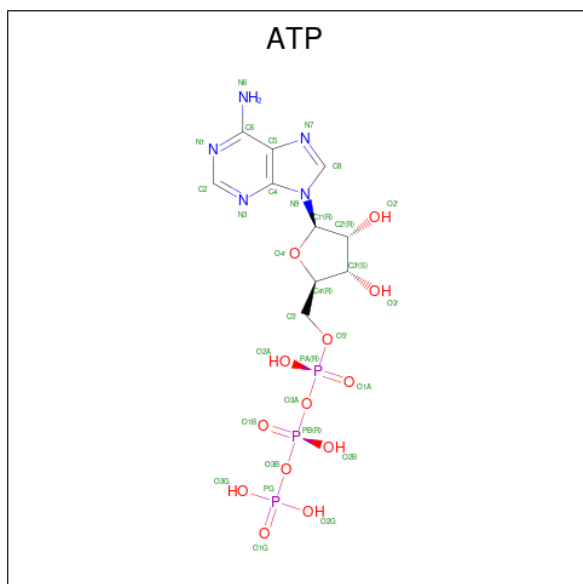
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT.

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 (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

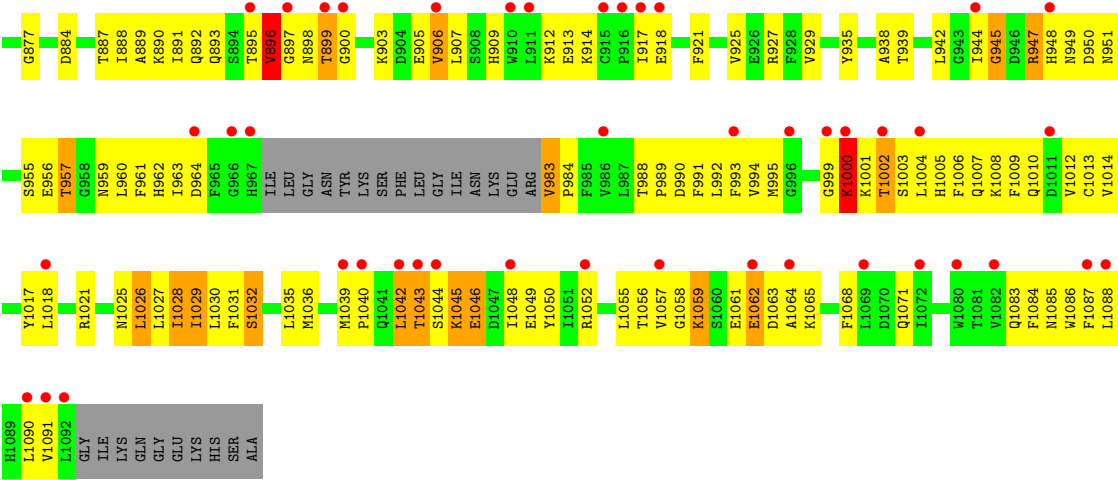


- Molecule 3 is LUTETIUM (III) ION (CCD ID: LU) (formula: Lu).

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, α , β , γ	143.29Å 67.56Å 106.95Å 90.00° 95.93° 90.00°	Depositor
Resolution (Å)	100.00 – 2.20 100.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.4 (100.00-2.20) 95.5 (100.00-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.255 , 0.306 0.238 , 0.292	Depositor DCC
R_{free} test set	5320 reflections (5.66%)	wwPDB-VP
Wilson B-factor (Å ²)	52.6	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.90	6/6946 (0.1%)	1.09	27/9396 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	842	MET	SD-CE	-9.08	1.56	1.79
1	A	664	VAL	CA-CB	6.16	1.62	1.54
1	A	198	MET	SD-CE	6.04	1.94	1.79
1	A	689	LYS	C-O	-5.20	1.18	1.24
1	A	703	ILE	CA-C	-5.15	1.45	1.52
1	A	697	TRP	CA-C	5.02	1.59	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	MET	N-CA-C	10.48	126.03	110.52
1	A	788	ASP	CA-C-N	9.20	129.80	119.32
1	A	788	ASP	C-N-CA	9.20	129.80	119.32
1	A	228	THR	N-CA-C	-8.84	102.51	113.20
1	A	165	VAL	N-CA-C	-8.12	105.22	113.10
1	A	387	ILE	N-CA-C	-7.11	97.62	107.99
1	A	554	GLN	N-CA-C	-7.10	104.49	113.72
1	A	555	LEU	N-CA-C	-6.72	104.02	111.82
1	A	503	THR	N-CA-C	6.51	119.92	110.28
1	A	604	VAL	N-CA-C	-6.48	104.01	110.62
1	A	609	GLN	N-CA-C	-6.37	103.59	112.45
1	A	945	GLY	N-CA-C	6.34	121.55	113.24
1	A	367	GLY	N-CA-C	6.28	119.73	110.63
1	A	738	VAL	N-CA-C	6.05	116.23	110.42
1	A	595	SER	N-CA-C	-5.74	105.47	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	644	ALA	N-CA-C	-5.66	105.03	111.14
1	A	470	ASP	N-CA-C	5.64	118.14	110.35
1	A	833	LYS	N-CA-C	5.49	118.41	109.24
1	A	694	PHE	N-CA-C	5.47	118.16	111.82
1	A	710	GLN	N-CA-C	5.30	117.06	111.28
1	A	429	LEU	N-CA-C	-5.27	99.19	108.20
1	A	406	GLU	N-CA-C	-5.26	107.23	113.97
1	A	678	ALA	N-CA-C	-5.25	105.55	111.28
1	A	513	SER	N-CA-C	5.24	117.62	110.55
1	A	695	LEU	N-CA-C	-5.19	105.62	111.28
1	A	1046	GLU	N-CA-C	-5.14	104.64	112.04
1	A	365	ILE	CB-CA-C	-5.01	104.94	111.81

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	445	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	445	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 32.

All (445) 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:804:MET:HE3	1:A:810:PRO:HB2	1.44	0.99
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:MET:HE1	1:A:938:ALA:CB	1.97	0.95
1:A:561:THR:HB	1:A:1025:ASN:HD21	1.36	0.89
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.38	0.88
1:A:804:MET:HE1	1:A:831:ILE:HD13	1.55	0.87
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: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:302:GLU:CD	1:A:304:HIS:HE2	1.91	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:181:VAL:HG12	1:A:185:MET:HE2	1.65	0.77
1:A:370:ILE:HD13	1:A:371:PRO:CD	2.14	0.77
1:A:778:ASN:N	1:A:778:ASN:HD22	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: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:641:ARG:HD3	1:A:670:GLU:CD	2.13	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: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
1:A:662:GLN:HE22	1:A:850:ILE:CD1	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:851:MET:HE1	1:A:938:ALA:HB2	1.72	0.71
1:A:853:SER:O	1:A:857:THR:HG23	1.90	0.71
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.72	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: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:995:MET:HE1	1:A:1009:PHE:HB2	1.72	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: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:851:MET:HE1	1:A:938:ALA:CA	2.26	0.66
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:804:MET:HE1	1:A:831:ILE:CD1	2.26	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:955:SER:C	1:A:957:THR:H	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:576:TRP:O	1:A:579:ARG:HG3	1.99	0.62
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.82	0.62
1:A:625:GLY:O	1:A:629:GLN:HG3	1.99	0.62
1:A:851:MET:HE1	1:A:938:ALA:HA	1.82	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:1062:GLU:CD	1:A:1062:GLU:H	2.09	0.61
1:A:989:PRO:HA	1:A:992:LEU:HD12	1.82	0.61
1:A:1084:PHE:CE2	1:A:1088:LEU:HD11	2.36	0.61
1:A:151:GLN:HA	1:A:154:LEU:HD12	1.81	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:799:GLU:CD	1:A:799:GLU:H	2.08	0.60
1:A:221:PHE:HD2	1:A:234:LYS:HG2	1.65	0.60
1:A:1049:GLU:HG3	1:A:1052:ARG:NH2	2.15	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:232:THR:C	1:A:233:ILE:HD12	2.26	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:772:GLU:HG2	1:A:798:ILE:HD13	1.85	0.59
1:A:1044:SER:C	1:A:1046:GLU:H	2.10	0.58
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:624:VAL:O	1:A:628:MET:HG2	2.04	0.57
1:A:187:GLU:OE2	1:A:687:ARG:HD3	2.04	0.57
1:A:470:ASP:OD1	1:A:472:ARG:N	2.37	0.57
1:A:808:LYS:HD2	1:A:835:GLY:HA3	1.85	0.57
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:HB3	1:A:947:ARG:NH1	2.19	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:251:LYS:HG2	1:A:252:MET:HE1	1.87	0.56
1:A:1044:SER:O	1:A:1046:GLU:N	2.39	0.56
1:A:393:VAL:HG23	1:A:393:VAL:O	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:777:LEU:C	1:A:778:ASN:HD22	2.14	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: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: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:750:LYS:HZ3	1:A:834:HIS:HD2	1.55	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:167:ASN:C	1:A:168:VAL:CG2	2.80	0.54
1:A:214:LYS:O	1:A:214:LYS:HG2	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:143:ALA:O	1:A:148:LEU:HD11	2.07	0.54
1:A:222:ILE:HG13	1:A:222:ILE:O	2.08	0.54
1:A:905:GLU:HB3	1:A:909:HIS:CE1	2.43	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:738:VAL:HG22	1:A:780:PRO:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1000:LYS:O	1:A:1000:LYS:HG2	2.07	0.53
1:A:899:THR:HG22	1:A:1087:PHE:HZ	1.73	0.53
1:A:1026:LEU:O	1:A:1029:ILE:HD12	2.08	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:187:GLU:CD	1:A:687:ARG:HG2	2.33	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:167:ASN:O	1:A:168:VAL:HG22	2.08	0.52
1:A:278:ASP:CG	1:A:784:ARG:HH22	2.17	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:274:VAL:HG23	1:A:279:GLU:O	2.09	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:602:GLU:CD	1:A:602:GLU:H	2.18	0.52
1:A:899:THR:HA	1:A:1087:PHE:CE2	2.44	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:215:ILE:C	1:A:217:ASN:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:217:ASN:O	1:A:218:ASN:HB2	2.11	0.51
1:A:563:PRO:HB2	1:A:1028:ILE:HG21	1.93	0.51
1:A:1061:GLU:HG3	1:A:1062:GLU:CD	2.36	0.51
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:528:ALA:O	1:A:529:LEU:HB2	2.09	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:552:ARG:HH21	1:A:578:PHE:HD1	1.58	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: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: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:929:VAL:HG22	1:A:995:MET:HE3	1.93	0.49
1:A:548:PRO:HB2	1:A:552:ARG:HD2	1.94	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: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:470:ASP:OD1	1:A:470:ASP:C	2.56	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:VAL:HG23	4:A:2119:HOH:O	2.13	0.49
1:A:558:ILE:C	1:A:560:ALA:H	2.20	0.48
1:A:583:LEU:C	1:A:585:ASP:H	2.21	0.48
1:A:851:MET:HE1	1:A:938:ALA:HB1	1.91	0.48
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: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:1021:ARG:HE	1:A:1056:THR:HG22	1.78	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:991:PHE:O	1:A:995:MET:HG3	2.14	0.48
1:A:180:LEU:C	1:A:183:PRO:HD2	2.39	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:1084:PHE:O	1:A:1088:LEU:HG	2.14	0.48
1:A:370:ILE:HD13	1:A:370:ILE:C	2.39	0.47
1:A:905:GLU:HB3	1:A:909:HIS:HD1	1.79	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:1035:LEU:HB3	1:A:1042:LEU:HD12	1.96	0.47
1:A:167:ASN:C	1:A:168:VAL:HG22	2.39	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:583:LEU:HD23	1:A:583:LEU:C	2.40	0.47
1:A:614:ARG:HB3	1:A:618:ASP:OD1	2.15	0.47
1:A:242:GLY:C	1:A:244:ILE:H	2.23	0.47
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.97	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:555:LEU:O	1:A:559:ILE:HG13	2.15	0.46
1:A:1001:LYS:O	1:A:1002:THR:C	2.58	0.46
1:A:1003:SER:HB2	1:A:1006:PHE:HB3	1.96	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:1052:ARG:O	1:A:1057:VAL:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ARG:HE	1:A:578:PHE:CB	2.28	0.46
1:A:851:MET:CE	1:A:938:ALA:HB2	2.44	0.46
1:A:472:ARG:O	1:A:473:PHE:HB2	2.14	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
1:A:658:HIS:HD2	4:A:2200:HOH:O	1.99	0.46
1:A:955:SER:C	1:A:957:THR:N	2.72	0.46
1:A:240:THR:C	4:A:2035:HOH:O	2.59	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:363:VAL:HG12	1:A:416:PHE:HE1	1.81	0.45
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:170:ASP:OD1	1:A:170:ASP:C	2.60	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: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:1014:VAL:CG1	1:A:1065:LYS:HG3	2.44	0.45
1:A:1044:SER:C	1:A:1046:GLU:N	2.75	0.45
1:A:659:TYR:HB2	4:A:2134:HOH:O	2.16	0.45
1:A:487:LEU:C	1:A:489:GLY:H	2.25	0.45
1:A:843:LEU:O	1:A:847:ILE:HD13	2.17	0.45
1:A:995:MET:CE	1:A:1009:PHE:HB2	2.43	0.45
1:A:154:LEU:O	1:A:158:ILE:HG12	2.16	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:806:SER:HB3	1:A:810:PRO:CD	2.47	0.44
1:A:1058:GLY:O	1:A:1059:LYS:C	2.60	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:HD12	1:A:233:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLY:C	1:A:244:ILE:N	2.76	0.44
1:A:287:ILE:HD12	1:A:287:ILE:C	2.42	0.44
1:A:196:TYR:OH	1:A:724:CYS:O	2.28	0.44
1:A:555:LEU:HD23	1:A:555:LEU:C	2.42	0.44
1:A:912:LYS:HG2	1:A:921:PHE:CE1	2.52	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:625:GLY:HA2	1:A:1026:LEU:HD23	1.98	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:549:ASN:H	1:A:549:ASN:HD22	1.65	0.44
1:A:750:LYS:HZ2	1:A:834:HIS:C	2.23	0.44
1:A:151:GLN:NE2	1:A:155:ASN:OD1	2.51	0.43
1:A:299:ASN:O	1:A:300:GLY:C	2.61	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:842:MET:HE2	1:A:871:SER:HB3	1.99	0.43
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.18	0.43
1:A:150:PHE:C	1:A:152:ARG:N	2.74	0.43
1:A:213:LYS:C	1:A:215:ILE:H	2.26	0.43
1:A:379:LEU:HD13	1:A:435:CYS:SG	2.59	0.43
1:A:1048:ILE:HG22	1:A:1048:ILE:O	2.18	0.43
1:A:1021:ARG:HH21	1:A:1056:THR:HG23	1.84	0.43
1:A:421:LYS:CE	1:A:526:PRO:HB3	2.48	0.43
1:A:586:PRO:C	1:A:588:ALA:H	2.27	0.43
1:A:586:PRO:O	1:A:588:ALA:N	2.52	0.43
1:A:884:ASP:OD1	1:A:884:ASP:O	2.37	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:217:ASN:C	1:A:219:CYS:H	2.26	0.43
1:A:276:GLY:HA2	1:A:819:ASP:CG	2.44	0.43
1:A:433:ILE:HG13	1:A:484:MET:HE1	2.01	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:196:TYR:OH	1:A:728:MET:HE2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:182:THR:CB	1:A:183:PRO:HD3	2.45	0.42
1:A:321:GLU:CD	1:A:321:GLU:N	2.77	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: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: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:847:ILE:HG22	1:A:848:LEU:N	2.35	0.42
1:A:487:LEU:C	1:A:489:GLY:N	2.77	0.42
1:A:804:MET:CE	1:A:810:PRO:HB2	2.32	0.42
1:A:376:THR:C	1:A:378:ASP:H	2.27	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: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: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:476:ARG:HE	1:A:476:ARG:HB2	1.44	0.41
1:A:738:VAL:CG2	1:A:780:PRO:HD2	2.50	0.41
1:A:1021:ARG:HE	1:A:1056:THR:CG2	2.33	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:1087:PHE:O	1:A:1087:PHE:HD1	2.03	0.41
1:A:546:GLU:O	1:A:547:MET:C	2.63	0.41
1:A:1035:LEU:HA	1:A:1039:MET:CG	2.51	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:498:ASN:OD1	1:A:498:ASN:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:LYS:HE3	1:A:756:LYS:HA	2.02	0.41
1:A:243:THR:HG22	1:A:243:THR:O	2.20	0.41
1:A:586:PRO:C	1:A:588:ALA:N	2.78	0.41
1:A:892:GLN:OE1	1:A:906:VAL:HG21	2.20	0.41
1:A:1000:LYS:HD3	1:A:1000:LYS:N	2.36	0.41
1:A:192:ASP:OD1	1:A:192:ASP:C	2.62	0.41
1:A:246:GLN:O	1:A:250:THR:HG23	2.20	0.41
1:A:268:ARG:H	1:A:268:ARG:HD3	1.86	0.41
1:A:274:VAL:CG2	1:A:279:GLU:HB3	2.51	0.41
1:A:633:CYS:SG	1:A:1036:MET:HE1	2.61	0.41
1:A:689:LYS:HG2	1:A:728:MET:HE2	2.02	0.41
1:A:1050:TYR:CD1	1:A:1050:TYR:C	2.99	0.41
1:A:1084:PHE:HE2	1:A:1088:LEU:HD11	1.84	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:929:VAL:HG22	1:A:995:MET:CE	2.51	0.40
1:A:316:ASP:O	1:A:317:GLU:C	2.64	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:899:THR:HA	1:A:1087:PHE:HZ	1.85	0.40
1:A:905:GLU:O	1:A:906:VAL:C	2.65	0.40
1:A:912:LYS:HA	1:A:921:PHE:CD1	2.56	0.40
1:A:947:ARG:NH1	1:A:947:ARG:CB	2.85	0.40
1:A:963:ILE:O	1:A:964:ASP:C	2.65	0.40
1:A:1061:GLU:O	1:A:1064:ALA:HB3	2.21	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%)	4 2

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%)	687 (91%)	69 (9%)	9 9

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	147	THR
1	A	165	VAL
1	A	168	VAL
1	A	173	LEU
1	A	179	ARG
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	240	THR
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	459	GLN
1	A	476	ARG
1	A	547	MET
1	A	555	LEU
1	A	575	LEU
1	A	616	VAL
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	770	LYS
1	A	775	GLN
1	A	778	ASN
1	A	791	LEU
1	A	792	LYS
1	A	807	LYS
1	A	823	LEU
1	A	838	LEU
1	A	843	LEU
1	A	844	ILE
1	A	845	LEU
1	A	848	LEU
1	A	888	ILE
1	A	890	LYS
1	A	896	VAL
1	A	899	THR
1	A	913	GLU
1	A	944	ILE
1	A	947	ARG
1	A	957	THR
1	A	960	LEU
1	A	983	VAL
1	A	988	THR
1	A	1000	LYS
1	A	1026	LEU
1	A	1027	LEU
1	A	1028	ILE
1	A	1029	ILE
1	A	1032	SER
1	A	1042	LEU
1	A	1043	THR
1	A	1062	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	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	601	GLN
1	A	619	GLN
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	1010	GLN
1	A	1025	ASN
1	A	1083	GLN
1	A	1089	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	32,33,33	2.29	3 (9%)	48,52,52	1.18	4 (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	-	-	1/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	ATP	PB-O3B	11.00	1.71	1.59
2	A	3000	ATP	PA-O3A	3.79	1.63	1.59
2	A	3000	ATP	PG-O2G	-2.03	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'	3.75	108.56	101.46
2	A	3000	ATP	O2A-PA-O3A	2.55	114.16	107.27
2	A	3000	ATP	O3A-PB-O1B	-2.19	104.11	110.70
2	A	3000	ATP	O3A-PA-O1A	-2.17	104.19	110.70

There are no chirality outliers.

All (1) torsion outliers are listed below:

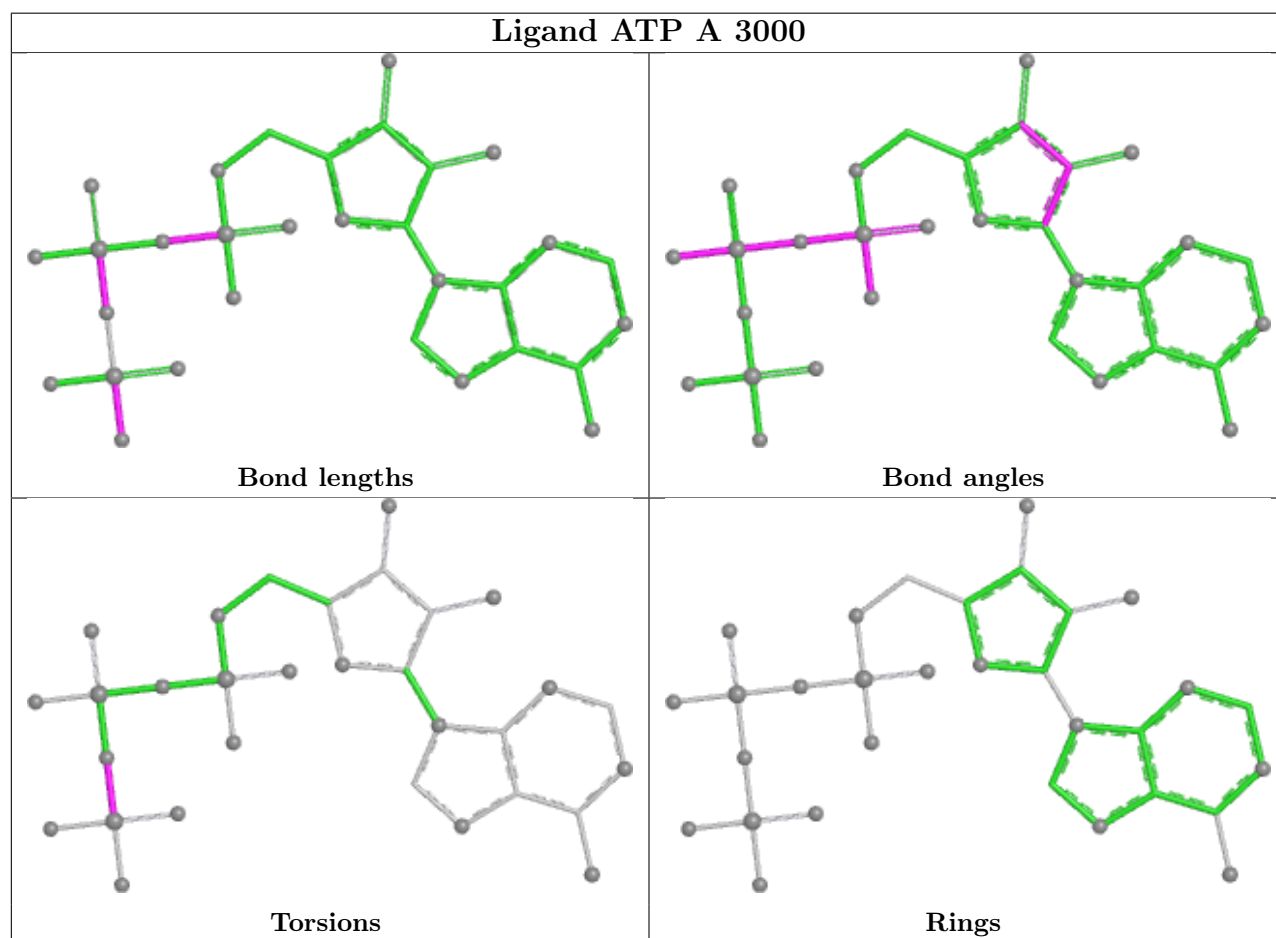
Mol	Chain	Res	Type	Atoms
2	A	3000	ATP	PB-O3B-PG-O3G

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

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, 95th 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 ²)	Q<0.9
1	A	841/961 (87%)	1.07	141 (16%) 4 3	24, 61, 98, 125	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	561	THR	5.3
1	A	211	LEU	5.1
1	A	379	LEU	4.8
1	A	210	TYR	4.7
1	A	552	ARG	4.6
1	A	752	LEU	4.3
1	A	245	LEU	4.2
1	A	283	GLY	4.2
1	A	527	ILE	4.0
1	A	143	ALA	3.8
1	A	147	THR	3.8
1	A	526	PRO	3.8
1	A	1040	PRO	3.8
1	A	241	PRO	3.8
1	A	1043	THR	3.7
1	A	917	ILE	3.7
1	A	1048	ILE	3.7
1	A	1042	LEU	3.7
1	A	215	ILE	3.5
1	A	1092	LEU	3.5
1	A	900	GLY	3.5
1	A	616	VAL	3.5
1	A	577	HIS	3.4
1	A	1004	LEU	3.4
1	A	551	LEU	3.3
1	A	617	TRP	3.3
1	A	249	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	966	GLY	3.2
1	A	270	PHE	3.2
1	A	142	ALA	3.2
1	A	996	GLY	3.2
1	A	148	LEU	3.2
1	A	560	ALA	3.1
1	A	1090	LEU	3.1
1	A	895	THR	3.0
1	A	986	VAL	3.0
1	A	214	LYS	3.0
1	A	999	GLY	3.0
1	A	964	ASP	3.0
1	A	548	PRO	2.9
1	A	474	LEU	2.9
1	A	168	VAL	2.9
1	A	181	VAL	2.9
1	A	253	ALA	2.9
1	A	777	LEU	2.9
1	A	1044	SER	2.9
1	A	282	VAL	2.9
1	A	222	ILE	2.8
1	A	208	PRO	2.8
1	A	167	ASN	2.8
1	A	757	TYR	2.8
1	A	1064	ALA	2.6
1	A	409	LEU	2.6
1	A	578	PHE	2.6
1	A	916	PRO	2.6
1	A	967	HIS	2.6
1	A	271	VAL	2.6
1	A	529	LEU	2.6
1	A	189	ALA	2.6
1	A	207	LEU	2.5
1	A	897	GLY	2.5
1	A	220	VAL	2.5
1	A	412	VAL	2.5
1	A	196	TYR	2.5
1	A	528	ALA	2.5
1	A	313	PRO	2.5
1	A	563	PRO	2.5
1	A	185	MET	2.4
1	A	175	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1087	PHE	2.4
1	A	1000	LYS	2.4
1	A	373	LEU	2.4
1	A	519	LEU	2.4
1	A	1062	GLU	2.4
1	A	564	LEU	2.4
1	A	358	ASP	2.4
1	A	753	SER	2.4
1	A	233	ILE	2.4
1	A	1072	ILE	2.4
1	A	1018	LEU	2.4
1	A	244	ILE	2.3
1	A	180	LEU	2.3
1	A	918	GLU	2.3
1	A	380	THR	2.3
1	A	405	THR	2.3
1	A	381	VAL	2.3
1	A	473	PHE	2.3
1	A	1091	VAL	2.3
1	A	193	PRO	2.3
1	A	401	PRO	2.3
1	A	899	THR	2.3
1	A	1082	VAL	2.3
1	A	1088	LEU	2.3
1	A	1039	MET	2.3
1	A	166	SER	2.3
1	A	1011	ASP	2.2
1	A	178	ARG	2.2
1	A	1052	ARG	2.2
1	A	240	THR	2.2
1	A	546	GLU	2.2
1	A	761	SER	2.2
1	A	910	TRP	2.2
1	A	305	LEU	2.2
1	A	487	LEU	2.2
1	A	248	PHE	2.2
1	A	948	HIS	2.2
1	A	307	LEU	2.2
1	A	522	ASN	2.2
1	A	547	MET	2.2
1	A	376	THR	2.2
1	A	751	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	559	ILE	2.2
1	A	759	VAL	2.2
1	A	778	ASN	2.2
1	A	825	ASN	2.2
1	A	1057	VAL	2.1
1	A	311	PRO	2.1
1	A	309	THR	2.1
1	A	520	LEU	2.1
1	A	555	LEU	2.1
1	A	911	LEU	2.1
1	A	171	ASP	2.1
1	A	525	HIS	2.1
1	A	221	PHE	2.1
1	A	250	THR	2.1
1	A	357	CYS	2.1
1	A	755	GLU	2.1
1	A	823	LEU	2.1
1	A	1069	LEU	2.1
1	A	558	ILE	2.1
1	A	906	VAL	2.1
1	A	1080	TRP	2.1
1	A	779	LEU	2.0
1	A	944	ILE	2.0
1	A	306	VAL	2.0
1	A	993	PHE	2.0
1	A	808	LYS	2.0
1	A	1002	THR	2.0
1	A	149	ALA	2.0
1	A	915	CYS	2.0
1	A	308	ASP	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 ⓘ

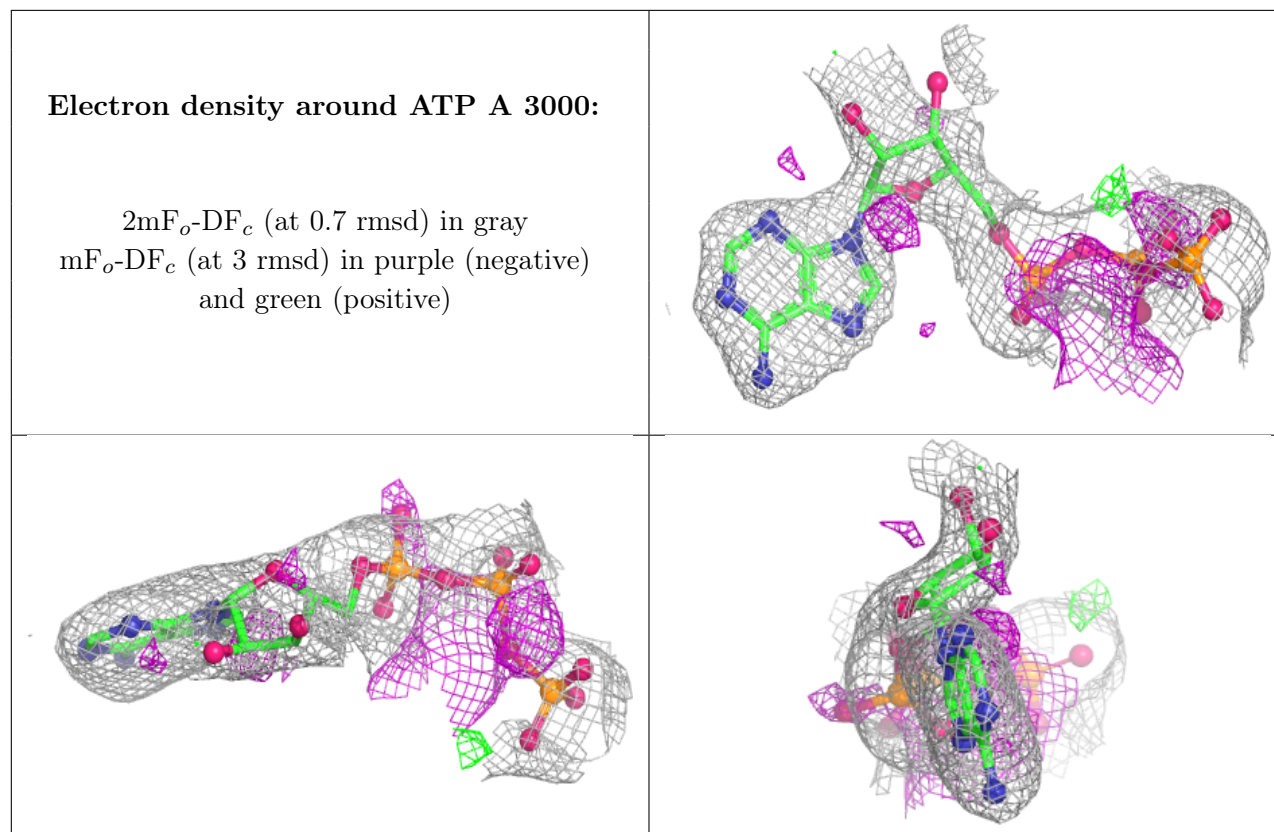
There are no oligosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	ATP	A	3000	31/31	0.86	0.14	66,80,92,93	0
3	LU	A	3009	1/1	0.91	0.10	135,135,135,135	0
3	LU	A	3007	1/1	0.93	0.08	121,121,121,121	0
3	LU	A	3001	1/1	0.95	0.08	72,72,72,72	0
3	LU	A	3002	1/1	0.95	0.08	70,70,70,70	0
3	LU	A	3006	1/1	0.97	0.11	86,86,86,86	0
3	LU	A	3003	1/1	0.97	0.09	76,76,76,76	0
3	LU	A	3008	1/1	0.97	0.11	108,108,108,108	0
3	LU	A	3004	1/1	0.97	0.11	72,72,72,72	0
3	LU	A	3005	1/1	0.98	0.08	77,77,77,77	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.