



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:18 PM UTC

PDB ID : 3LMI / pdb_00003lmi
Title : Crystal Structure of the Inactive Alpha-kinase Domain of Myosin Heavy Chain Kinase A (D766A) complex with ATP
Authors : Ye, Q.; Jia, Z.
Deposited on : 2010-01-30
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

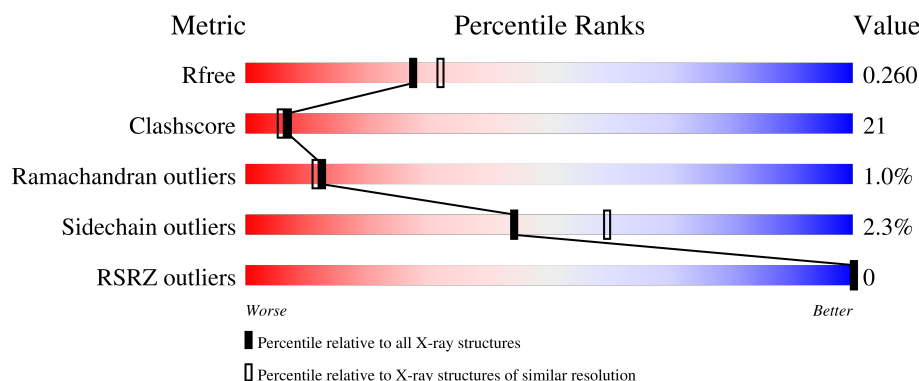
1 Overall quality at a glance

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	307	
1	B	307	
1	C	307	
1	D	307	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8689 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 Myosin heavy chain kinase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1953	1256	329	356	12			
1	B	254	Total	C	N	O	S	0	0	0
			2012	1291	338	371	12			
1	C	250	Total	C	N	O	S	0	0	0
			1986	1276	334	364	12			
1	D	253	Total	C	N	O	S	0	0	0
			2005	1287	335	371	12			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	MET	-	expression tag	UNP P42527
A	536	GLY	-	expression tag	UNP P42527
A	537	GLY	-	expression tag	UNP P42527
A	538	HIS	-	expression tag	UNP P42527
A	539	HIS	-	expression tag	UNP P42527
A	540	HIS	-	expression tag	UNP P42527
A	541	HIS	-	expression tag	UNP P42527
A	542	HIS	-	expression tag	UNP P42527
A	543	HIS	-	expression tag	UNP P42527
A	544	GLY	-	expression tag	UNP P42527
A	545	GLU	-	expression tag	UNP P42527
A	546	ASN	-	expression tag	UNP P42527
A	547	LEU	-	expression tag	UNP P42527
A	548	TYR	-	expression tag	UNP P42527
A	549	PHE	-	expression tag	UNP P42527
A	550	GLN	-	expression tag	UNP P42527
A	551	GLY	-	expression tag	UNP P42527
A	766	ALA	ASP	engineered mutation	UNP P42527
B	535	MET	-	expression tag	UNP P42527
B	536	GLY	-	expression tag	UNP P42527
B	537	GLY	-	expression tag	UNP P42527

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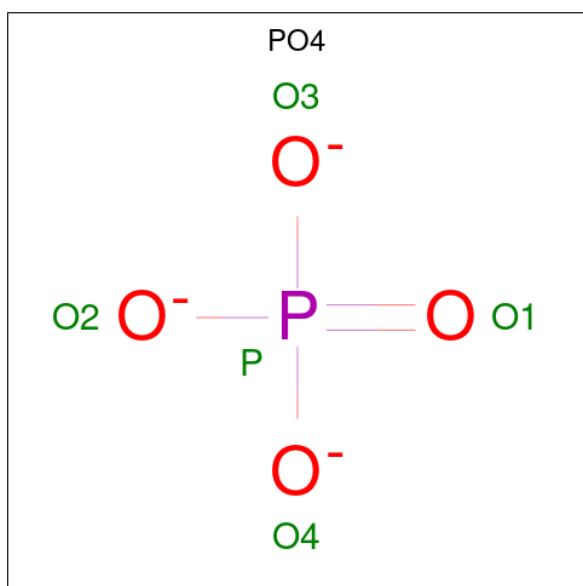
Chain	Residue	Modelled	Actual	Comment	Reference
B	538	HIS	-	expression tag	UNP P42527
B	539	HIS	-	expression tag	UNP P42527
B	540	HIS	-	expression tag	UNP P42527
B	541	HIS	-	expression tag	UNP P42527
B	542	HIS	-	expression tag	UNP P42527
B	543	HIS	-	expression tag	UNP P42527
B	544	GLY	-	expression tag	UNP P42527
B	545	GLU	-	expression tag	UNP P42527
B	546	ASN	-	expression tag	UNP P42527
B	547	LEU	-	expression tag	UNP P42527
B	548	TYR	-	expression tag	UNP P42527
B	549	PHE	-	expression tag	UNP P42527
B	550	GLN	-	expression tag	UNP P42527
B	551	GLY	-	expression tag	UNP P42527
B	766	ALA	ASP	engineered mutation	UNP P42527
C	535	MET	-	expression tag	UNP P42527
C	536	GLY	-	expression tag	UNP P42527
C	537	GLY	-	expression tag	UNP P42527
C	538	HIS	-	expression tag	UNP P42527
C	539	HIS	-	expression tag	UNP P42527
C	540	HIS	-	expression tag	UNP P42527
C	541	HIS	-	expression tag	UNP P42527
C	542	HIS	-	expression tag	UNP P42527
C	543	HIS	-	expression tag	UNP P42527
C	544	GLY	-	expression tag	UNP P42527
C	545	GLU	-	expression tag	UNP P42527
C	546	ASN	-	expression tag	UNP P42527
C	547	LEU	-	expression tag	UNP P42527
C	548	TYR	-	expression tag	UNP P42527
C	549	PHE	-	expression tag	UNP P42527
C	550	GLN	-	expression tag	UNP P42527
C	551	GLY	-	expression tag	UNP P42527
C	766	ALA	ASP	engineered mutation	UNP P42527
D	535	MET	-	expression tag	UNP P42527
D	536	GLY	-	expression tag	UNP P42527
D	537	GLY	-	expression tag	UNP P42527
D	538	HIS	-	expression tag	UNP P42527
D	539	HIS	-	expression tag	UNP P42527
D	540	HIS	-	expression tag	UNP P42527
D	541	HIS	-	expression tag	UNP P42527
D	542	HIS	-	expression tag	UNP P42527
D	543	HIS	-	expression tag	UNP P42527

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Chain	Residue	Modelled	Actual	Comment	Reference
D	544	GLY	-	expression tag	UNP P42527
D	545	GLU	-	expression tag	UNP P42527
D	546	ASN	-	expression tag	UNP P42527
D	547	LEU	-	expression tag	UNP P42527
D	548	TYR	-	expression tag	UNP P42527
D	549	PHE	-	expression tag	UNP P42527
D	550	GLN	-	expression tag	UNP P42527
D	551	GLY	-	expression tag	UNP P42527
D	766	ALA	ASP	engineered mutation	UNP P42527

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

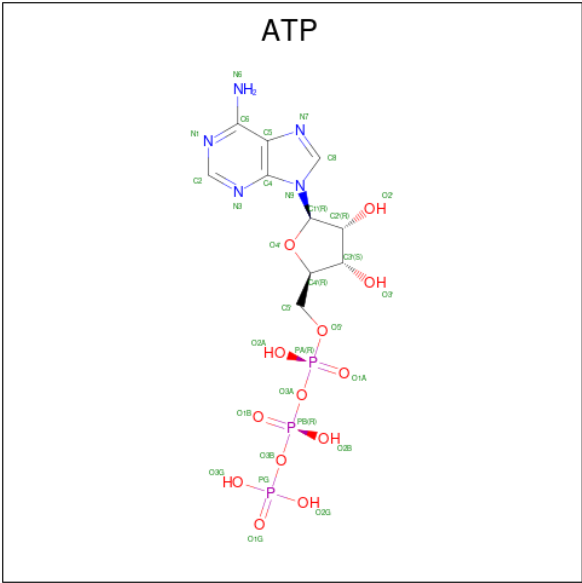
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

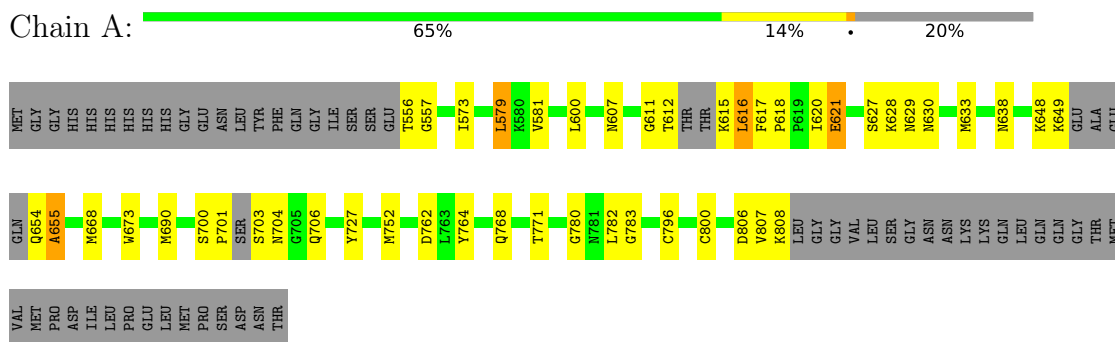
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	130	Total	O	0	0
			130	130		
6	B	153	Total	O	0	0
			153	153		
6	C	138	Total	O	0	0
			138	138		
6	D	150	Total	O	0	0
			150	150		

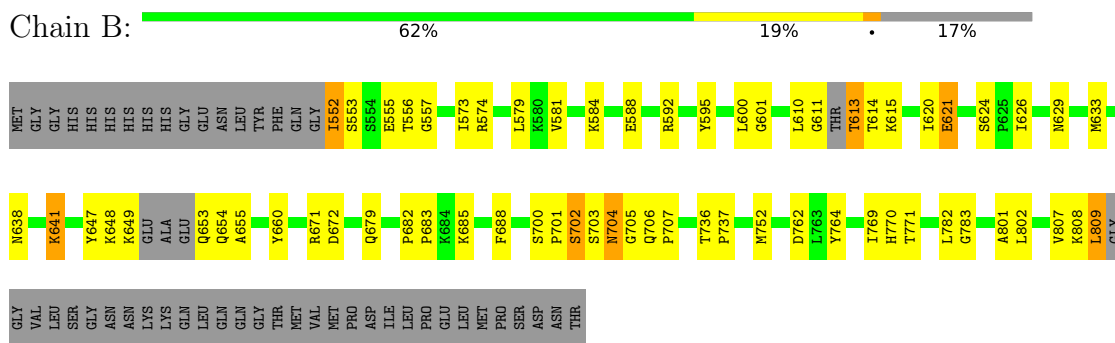
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

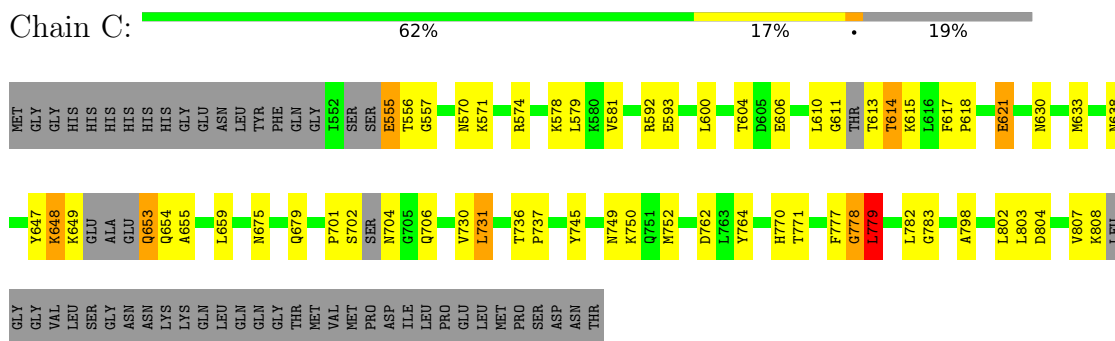
• Molecule 1: Myosin heavy chain kinase A



• Molecule 1: Myosin heavy chain kinase A

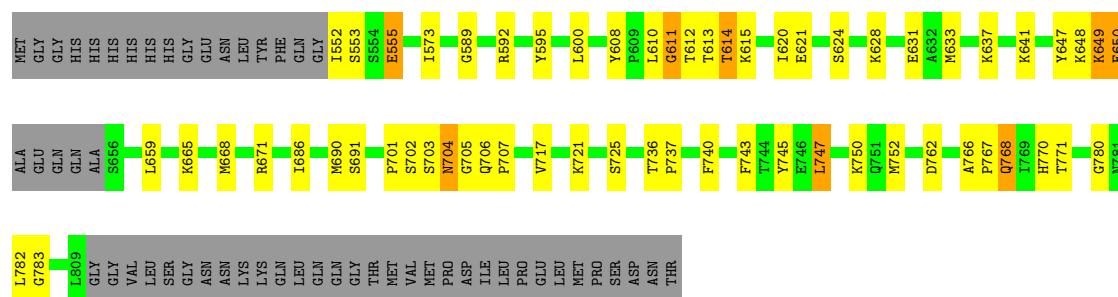


• Molecule 1: Myosin heavy chain kinase A



• Molecule 1: Myosin heavy chain kinase A

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	81.19Å 81.19Å 187.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.17 – 2.20 29.17 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.2 (29.17-2.20) 92.2 (29.17-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.24 (at 2.20Å)	Xtriage
Refinement program	REFMAC 6.1.0	Depositor
R, R_{free}	0.199 , 0.269 0.196 , 0.260	Depositor DCC
R_{free} test set	2863 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8689	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.31% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ZN, 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	0.63	0/1994	0.83	1/2687 (0.0%)
1	B	0.68	0/2054	0.82	1/2770 (0.0%)
1	C	0.62	0/2026	0.84	2/2729 (0.1%)
1	D	0.70	0/2048	0.84	3/2764 (0.1%)
All	All	0.66	0/8122	0.83	7/10950 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	616	LEU	N-CA-C	6.97	120.48	110.24
1	C	779	LEU	N-CA-C	6.18	118.82	111.71
1	C	614	THR	CB-CA-C	-6.08	109.55	116.54
1	B	592	ARG	N-CA-C	5.36	117.82	109.52
1	D	608	TYR	CA-C-N	5.14	125.38	119.83
1	D	608	TYR	C-N-CA	5.14	125.38	119.83
1	D	592	ARG	N-CA-C	5.11	117.43	109.52

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	1953	0	1982	59	1
1	B	2012	0	2040	98	1
1	C	1986	0	2013	105	0
1	D	2005	0	2033	77	0
2	A	5	0	0	0	0
2	B	10	0	0	1	0
2	C	5	0	0	0	0
2	D	10	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	0	12	0	0
5	B	31	0	12	2	0
5	C	31	0	12	2	0
5	D	31	0	12	3	0
6	A	130	0	0	20	0
6	B	153	0	0	29	0
6	C	138	0	0	11	0
6	D	150	0	0	27	0
All	All	8689	0	8116	343	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 21.

All (343) 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:B:649:LYS:CD	1:B:653:GLN:N	1.76	1.48
1:D:631:GLU:HG3	1:D:690:MET:CE	1.57	1.34
1:B:613:THR:CG2	1:B:614:THR:H	1.37	1.34
1:B:660:TYR:CD1	6:B:344:HOH:O	1.79	1.34
1:B:648:LYS:O	1:B:649:LYS:HG2	1.18	1.29
1:B:629:ASN:HB3	6:B:278:HOH:O	1.38	1.23
1:C:633:MET:HE3	6:C:404:HOH:O	1.38	1.22
1:D:690:MET:SD	6:D:852:HOH:O	1.95	1.21
1:B:584:LYS:HE3	6:B:369:HOH:O	1.36	1.18
1:C:648:LYS:O	1:C:653:GLN:CG	1.92	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:MET:SD	6:A:478:HOH:O	2.02	1.17
1:D:631:GLU:CG	1:D:690:MET:HE3	1.74	1.16
1:B:649:LYS:HD2	1:B:653:GLN:N	0.82	1.14
1:B:613:THR:CG2	1:B:614:THR:N	2.01	1.13
1:B:648:LYS:O	1:B:649:LYS:CG	1.96	1.11
1:B:707:PRO:HD3	6:B:347:HOH:O	0.95	1.11
1:D:752:MET:HG3	6:D:479:HOH:O	0.94	1.10
1:A:704:ASN:OD1	1:A:706:GLN:HG2	1.51	1.10
1:B:641:LYS:NZ	6:B:262:HOH:O	1.87	1.08
1:B:584:LYS:CE	6:B:369:HOH:O	1.95	1.07
1:D:628:LYS:HE2	6:D:491:HOH:O	1.54	1.06
1:C:648:LYS:O	1:C:653:GLN:HG2	1.50	1.06
1:B:611:GLY:C	1:B:613:THR:CG2	2.28	1.06
1:B:633:MET:HG2	6:B:222:HOH:O	1.57	1.04
1:D:620:ILE:CG2	1:D:621:GLU:OE2	2.07	1.03
1:C:802:LEU:CD1	6:C:297:HOH:O	2.04	1.03
1:B:679:GLN:HB3	6:B:845:HOH:O	0.84	1.02
1:D:620:ILE:HG22	1:D:621:GLU:OE2	1.57	1.01
1:D:768:GLN:HG2	6:D:413:HOH:O	1.60	1.01
1:C:613:THR:HG22	1:C:614:THR:H	1.25	1.00
1:B:613:THR:HG22	1:B:614:THR:N	1.65	1.00
1:C:659:LEU:HD11	1:C:779:LEU:CD2	1.92	1.00
1:C:648:LYS:O	1:C:653:GLN:HG3	1.61	0.99
1:D:648:LYS:O	1:D:649:LYS:HG3	1.62	0.99
1:D:614:THR:HG22	1:D:614:THR:O	1.58	0.99
1:B:613:THR:HG23	1:B:614:THR:N	1.79	0.97
1:D:615:LYS:HG2	6:D:428:HOH:O	1.62	0.97
1:B:611:GLY:C	1:B:613:THR:HG22	1.90	0.97
1:B:613:THR:HG22	1:B:614:THR:H	0.81	0.96
1:A:620:ILE:CG2	6:A:214:HOH:O	2.13	0.96
1:A:620:ILE:HG22	6:A:214:HOH:O	1.65	0.96
1:C:655:ALA:HB3	1:C:659:LEU:HD23	1.48	0.96
1:A:628:LYS:HE3	6:A:378:HOH:O	1.65	0.95
1:D:768:GLN:NE2	6:D:477:HOH:O	2.01	0.94
1:B:700:SER:C	1:B:702:SER:H	1.75	0.94
1:C:802:LEU:HD11	6:C:297:HOH:O	1.66	0.92
1:A:633:MET:HE3	6:A:844:HOH:O	1.68	0.92
1:B:614:THR:HG22	1:B:615:LYS:H	1.35	0.92
1:C:659:LEU:CD2	1:C:779:LEU:HD21	2.00	0.92
1:C:659:LEU:CD1	1:C:779:LEU:CD2	2.48	0.91
1:A:704:ASN:OD1	1:A:706:GLN:CG	2.18	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:GLY:HA2	6:B:846:HOH:O	1.71	0.90
1:D:633:MET:HG2	6:D:259:HOH:O	1.72	0.88
1:B:611:GLY:C	1:B:613:THR:HG21	1.96	0.87
1:B:770:HIS:HD2	1:B:782:LEU:H	1.17	0.86
1:B:682:PRO:HD2	1:B:685:LYS:HE2	1.57	0.86
1:B:809:LEU:N	1:B:809:LEU:HD23	1.91	0.86
1:C:798:ALA:O	1:C:802:LEU:HD13	1.74	0.86
1:D:610:LEU:O	1:D:611:GLY:O	1.94	0.86
1:B:660:TYR:CE1	6:B:233:HOH:O	2.29	0.86
1:D:770:HIS:HD2	1:D:782:LEU:H	1.24	0.86
1:A:612:THR:HB	1:A:616:LEU:HG	1.58	0.85
1:C:659:LEU:CD1	1:C:779:LEU:HD21	2.07	0.85
1:B:649:LYS:HE2	1:B:654:GLN:N	1.92	0.84
1:C:600:LEU:HA	1:C:638:ASN:ND2	1.93	0.84
1:C:593:GLU:OE2	1:C:649:LYS:HE3	1.78	0.83
1:C:655:ALA:HB3	1:C:659:LEU:CD2	2.10	0.82
1:A:630:ASN:OD1	1:A:633:MET:HG2	1.79	0.82
1:B:629:ASN:CB	6:B:278:HOH:O	2.08	0.82
1:C:655:ALA:CB	1:C:659:LEU:CD2	2.59	0.81
1:C:600:LEU:C	1:C:638:ASN:HD22	1.89	0.81
1:B:700:SER:O	1:B:702:SER:N	2.13	0.80
1:B:629:ASN:OD1	6:B:278:HOH:O	1.99	0.80
1:B:588:GLU:OE1	1:B:648:LYS:NZ	2.14	0.80
1:D:631:GLU:HG3	1:D:690:MET:HE3	0.85	0.80
1:C:648:LYS:C	1:C:653:GLN:HG2	2.07	0.80
1:C:556:THR:HG22	6:C:850:HOH:O	1.80	0.79
1:B:770:HIS:CD2	1:B:782:LEU:H	1.99	0.79
1:B:614:THR:HG22	1:B:615:LYS:N	1.96	0.79
1:D:620:ILE:HG23	1:D:621:GLU:OE2	1.83	0.79
1:D:614:THR:O	1:D:614:THR:CG2	2.32	0.78
1:A:630:ASN:HD21	1:A:633:MET:HE2	1.46	0.78
1:B:660:TYR:CE1	6:B:344:HOH:O	2.17	0.78
1:D:613:THR:C	6:D:428:HOH:O	2.26	0.78
1:C:706:GLN:OE1	1:C:706:GLN:HA	1.83	0.77
1:D:752:MET:CG	6:D:479:HOH:O	1.73	0.76
1:C:770:HIS:HD2	1:C:782:LEU:H	1.34	0.76
1:D:770:HIS:CD2	1:D:782:LEU:H	2.04	0.75
1:B:660:TYR:HD1	6:B:344:HOH:O	1.35	0.75
1:A:648:LYS:O	1:A:649:LYS:C	2.30	0.74
1:D:768:GLN:CG	6:D:413:HOH:O	2.27	0.74
1:C:574:ARG:CZ	1:C:610:LEU:HD12	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:LYS:HE2	1:B:654:GLN:H	1.49	0.73
1:D:752:MET:CE	6:D:479:HOH:O	2.34	0.73
1:C:655:ALA:CB	1:C:659:LEU:HD22	2.17	0.73
1:D:703:SER:O	1:D:704:ASN:CB	2.35	0.73
1:D:762:ASP:OD2	6:D:356:HOH:O	2.05	0.73
1:A:654:GLN:CG	6:A:376:HOH:O	2.36	0.73
1:B:700:SER:C	1:B:702:SER:N	2.44	0.73
1:D:706:GLN:HA	1:D:706:GLN:OE1	1.87	0.72
1:A:649:LYS:O	1:A:649:LYS:HG3	1.88	0.72
1:D:705:GLY:O	6:D:418:HOH:O	2.05	0.72
1:D:589:GLY:HA3	5:D:1763:ATP:O1B	1.88	0.72
6:B:206:HOH:O	1:D:641:LYS:HE2	1.89	0.72
1:A:654:GLN:HG3	1:A:655:ALA:H	1.53	0.72
1:A:654:GLN:HG3	6:A:376:HOH:O	1.90	0.71
1:C:659:LEU:HD21	1:C:779:LEU:HD21	1.72	0.71
1:D:752:MET:HE2	6:D:479:HOH:O	1.89	0.71
1:A:654:GLN:CG	1:A:655:ALA:H	2.03	0.71
1:C:770:HIS:CD2	1:C:782:LEU:H	2.08	0.71
5:B:1761:ATP:O3G	5:B:1761:ATP:O2B	2.08	0.70
1:C:600:LEU:C	1:C:638:ASN:ND2	2.49	0.70
1:C:779:LEU:N	1:C:779:LEU:HD22	2.06	0.70
1:D:668:MET:HE3	6:D:15:HOH:O	1.90	0.70
1:C:679:GLN:NE2	6:C:315:HOH:O	2.25	0.69
1:C:555:GLU:O	1:C:578:LYS:CE	2.40	0.69
1:C:615:LYS:HE3	1:C:617:PHE:HB2	1.73	0.69
1:C:613:THR:HG22	1:C:614:THR:N	2.04	0.69
1:C:648:LYS:HA	1:C:649:LYS:HB2	1.74	0.69
1:D:721:LYS:NZ	6:D:851:HOH:O	2.24	0.69
1:C:555:GLU:HB2	6:C:503:HOH:O	1.92	0.68
1:B:641:LYS:HE3	1:D:717:VAL:HG23	1.74	0.68
1:B:771:THR:O	1:B:783:GLY:HA2	1.94	0.67
1:D:668:MET:HE1	1:D:691:SER:H	1.60	0.67
1:B:621:GLU:CD	1:B:621:GLU:H	2.04	0.66
1:C:655:ALA:HB2	1:C:659:LEU:HD22	1.77	0.66
1:D:611:GLY:HA3	6:D:498:HOH:O	1.94	0.66
1:D:745:TYR:CZ	1:D:750:LYS:HG2	2.29	0.66
1:A:579:LEU:HG	6:A:238:HOH:O	1.96	0.66
1:C:610:LEU:O	1:C:611:GLY:C	2.39	0.66
1:A:579:LEU:C	1:A:579:LEU:HD12	2.20	0.66
1:C:579:LEU:C	1:C:579:LEU:HD12	2.19	0.66
1:B:611:GLY:O	1:B:613:THR:CG2	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:LEU:HD11	1:C:779:LEU:HD23	1.78	0.66
1:D:768:GLN:OE1	6:D:413:HOH:O	2.13	0.65
1:C:704:ASN:OD1	1:C:706:GLN:HG2	1.97	0.65
1:D:555:GLU:OE1	1:D:600:LEU:HG	1.96	0.65
1:B:660:TYR:HE1	6:B:233:HOH:O	1.73	0.65
1:B:683:PRO:HD3	1:B:802:LEU:HD13	1.79	0.65
1:B:707:PRO:CD	6:B:347:HOH:O	1.77	0.65
1:A:673:TRP:NE1	1:A:752:MET:HE1	2.12	0.64
1:C:600:LEU:CA	1:C:638:ASN:ND2	2.59	0.64
1:D:650:GLU:N	1:D:650:GLU:OE2	2.31	0.64
1:B:649:LYS:CE	1:B:653:GLN:N	2.60	0.63
1:B:809:LEU:N	1:B:809:LEU:CD2	2.61	0.63
1:C:600:LEU:HA	1:C:638:ASN:HD21	1.62	0.63
1:D:648:LYS:O	1:D:649:LYS:CG	2.43	0.63
1:C:579:LEU:HD12	1:C:579:LEU:O	1.98	0.63
1:C:574:ARG:CZ	1:C:610:LEU:CD1	2.77	0.63
1:C:802:LEU:HD12	6:C:504:HOH:O	1.97	0.63
1:B:611:GLY:O	1:B:613:THR:HB	1.99	0.62
1:B:614:THR:CG2	1:B:615:LYS:H	2.09	0.62
1:C:762:ASP:OD1	1:C:764:TYR:OH	2.12	0.62
6:A:252:HOH:O	1:B:626:ILE:CD1	2.46	0.62
1:D:771:THR:O	1:D:783:GLY:HA2	1.99	0.62
1:B:600:LEU:HA	1:B:638:ASN:HD22	1.65	0.62
1:A:654:GLN:HG2	6:A:376:HOH:O	1.99	0.62
1:B:600:LEU:HA	1:B:638:ASN:ND2	2.14	0.62
1:C:771:THR:O	1:C:783:GLY:HA2	1.99	0.62
1:B:802:LEU:O	1:B:802:LEU:HD23	1.99	0.62
1:B:649:LYS:NZ	1:B:655:ALA:HB2	2.15	0.61
1:B:682:PRO:HD2	1:B:685:LYS:CE	2.26	0.61
1:C:555:GLU:O	1:C:578:LYS:NZ	2.33	0.61
1:A:620:ILE:HG23	6:A:214:HOH:O	1.87	0.61
1:B:649:LYS:HZ1	1:B:655:ALA:HB2	1.65	0.61
1:B:704:ASN:OD1	1:B:706:GLN:HG2	2.00	0.61
1:B:633:MET:HB2	6:B:294:HOH:O	2.00	0.61
1:B:641:LYS:HE2	6:D:159:HOH:O	2.00	0.61
5:C:1762:ATP:O1A	5:C:1762:ATP:O1B	2.17	0.61
1:D:573:ILE:HD13	1:D:624:SER:HB3	1.82	0.60
1:A:600:LEU:HA	1:A:638:ASN:ND2	2.16	0.60
1:A:654:GLN:HG3	1:A:655:ALA:N	2.16	0.60
1:C:745:TYR:CE2	1:C:750:LYS:HD2	2.37	0.59
1:A:771:THR:O	1:A:783:GLY:HA2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:LEU:HD13	1:C:779:LEU:CD2	2.31	0.59
1:A:701:PRO:O	1:A:703:SER:N	2.35	0.59
1:C:779:LEU:HD22	1:C:779:LEU:H	1.68	0.59
1:C:675:ASN:O	1:C:679:GLN:HG3	2.04	0.58
1:B:648:LYS:O	1:B:649:LYS:CB	2.52	0.58
1:D:668:MET:CE	1:D:691:SER:H	2.15	0.58
1:D:703:SER:O	1:D:704:ASN:HB2	2.02	0.58
1:A:654:GLN:CG	1:A:655:ALA:N	2.66	0.58
1:C:610:LEU:O	1:C:611:GLY:O	2.21	0.58
1:C:779:LEU:CD2	1:C:779:LEU:H	2.17	0.58
1:B:552:ILE:HB	1:B:601:GLY:HA3	1.86	0.58
1:D:707:PRO:HD3	6:D:418:HOH:O	2.03	0.58
1:A:806:ASP:OD2	1:A:808:LYS:HB2	2.04	0.58
1:A:621:GLU:N	6:A:214:HOH:O	2.28	0.57
1:A:629:ASN:HB2	6:A:378:HOH:O	2.04	0.57
1:C:649:LYS:H	1:C:653:GLN:CD	2.12	0.57
1:B:629:ASN:CG	6:B:278:HOH:O	2.31	0.57
1:B:752:MET:HE3	1:B:769:ILE:HD13	1.87	0.57
1:A:556:THR:HG23	1:A:557:GLY:N	2.20	0.57
1:B:641:LYS:HE3	1:D:717:VAL:CG2	2.34	0.57
1:C:574:ARG:CD	1:C:610:LEU:HD11	2.35	0.57
1:B:552:ILE:N	6:B:392:HOH:O	2.36	0.56
1:D:613:THR:HG22	1:D:613:THR:O	2.05	0.56
1:A:654:GLN:HA	1:A:654:GLN:OE1	2.06	0.56
1:C:613:THR:C	1:C:614:THR:HG22	2.29	0.56
1:D:649:LYS:C	1:D:650:GLU:OE2	2.49	0.56
1:B:647:TYR:HD1	6:B:233:HOH:O	1.88	0.56
1:C:648:LYS:C	1:C:653:GLN:CG	2.71	0.56
1:B:679:GLN:CG	6:B:845:HOH:O	2.32	0.55
1:C:614:THR:OG1	1:C:615:LYS:N	2.37	0.55
1:A:796:CYS:HB2	1:A:800:CYS:CB	2.36	0.55
1:D:707:PRO:HG2	6:D:343:HOH:O	2.05	0.55
1:C:659:LEU:CD1	1:C:779:LEU:HD22	2.35	0.55
1:C:617:PHE:HA	1:C:618:PRO:C	2.30	0.55
1:D:665:LYS:HE2	6:D:848:HOH:O	2.06	0.55
1:D:703:SER:O	1:D:704:ASN:HB3	2.06	0.55
1:A:649:LYS:O	1:A:649:LYS:CG	2.54	0.55
1:A:654:GLN:NE2	6:A:464:HOH:O	2.39	0.54
1:B:704:ASN:OD1	1:B:704:ASN:C	2.49	0.54
6:A:252:HOH:O	1:B:626:ILE:HD11	2.06	0.54
1:A:600:LEU:HA	1:A:638:ASN:HD22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:GLN:HA	1:A:706:GLN:OE1	2.07	0.54
1:C:571:LYS:HE2	6:C:182:HOH:O	2.07	0.54
1:A:617:PHE:HA	1:A:618:PRO:C	2.32	0.54
1:B:762:ASP:HA	1:B:764:TYR:CZ	2.43	0.54
1:C:779:LEU:CD2	1:C:779:LEU:N	2.70	0.54
1:C:731:LEU:N	1:C:731:LEU:HD12	2.23	0.54
1:D:736:THR:HB	1:D:737:PRO:HD3	1.90	0.53
1:A:581:VAL:HG12	6:A:23:HOH:O	2.07	0.53
1:B:611:GLY:O	1:B:613:THR:HG22	2.08	0.53
1:B:802:LEU:HD23	1:B:802:LEU:C	2.32	0.53
1:B:703:SER:C	1:B:705:GLY:H	2.15	0.53
1:B:621:GLU:N	1:B:621:GLU:OE1	2.42	0.53
1:D:768:GLN:CD	6:D:413:HOH:O	2.50	0.52
1:B:595:TYR:CE1	2:B:5959:PO4:O3	2.62	0.52
1:B:672:ASP:OD2	6:B:509:HOH:O	2.18	0.52
1:C:659:LEU:HD22	1:C:779:LEU:HD21	1.84	0.52
1:C:655:ALA:CB	1:C:659:LEU:HD23	2.24	0.52
1:A:556:THR:HG23	1:A:557:GLY:H	1.74	0.52
1:B:584:LYS:NZ	6:B:369:HOH:O	2.31	0.51
1:A:607:ASN:ND2	6:A:424:HOH:O	2.43	0.51
1:D:595:TYR:CE1	2:D:5960:PO4:O1	2.63	0.51
1:D:704:ASN:OD1	1:D:706:GLN:HG2	2.10	0.51
1:B:653:GLN:HA	1:B:653:GLN:OE1	2.09	0.51
1:A:704:ASN:OD1	1:A:706:GLN:CB	2.59	0.51
1:D:552:ILE:CG2	1:D:553:SER:N	2.73	0.51
1:C:807:VAL:HG22	1:C:808:LYS:N	2.24	0.51
1:D:725:SER:HB2	6:D:185:HOH:O	2.11	0.51
1:A:768:GLN:NE2	1:A:780:GLY:H	2.08	0.50
1:C:633:MET:CE	6:C:404:HOH:O	2.21	0.50
1:D:631:GLU:CG	1:D:690:MET:CE	2.54	0.50
1:B:611:GLY:O	1:B:613:THR:CB	2.59	0.50
1:D:631:GLU:CB	1:D:690:MET:HE3	2.40	0.50
1:C:570:ASN:O	1:C:571:LYS:HG2	2.11	0.50
1:B:679:GLN:CB	6:B:845:HOH:O	1.71	0.49
1:C:701:PRO:O	1:C:702:SER:C	2.56	0.49
1:B:707:PRO:HG2	6:B:385:HOH:O	2.11	0.49
1:A:654:GLN:CD	1:A:655:ALA:H	2.20	0.49
1:C:556:THR:O	1:C:556:THR:HG23	2.11	0.49
1:C:648:LYS:HA	1:C:649:LYS:CB	2.39	0.48
1:D:621:GLU:CD	1:D:621:GLU:H	2.21	0.48
1:C:579:LEU:C	1:C:579:LEU:CD1	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:ARG:HD3	1:C:610:LEU:HD11	1.95	0.48
1:D:610:LEU:C	1:D:611:GLY:O	2.57	0.48
1:D:745:TYR:CE2	1:D:750:LYS:HG2	2.49	0.48
1:A:768:GLN:NE2	6:A:293:HOH:O	2.36	0.48
1:B:808:LYS:C	1:B:809:LEU:HD23	2.39	0.48
1:D:768:GLN:NE2	1:D:780:GLY:C	2.72	0.48
1:C:807:VAL:CG2	1:C:808:LYS:N	2.76	0.48
1:D:768:GLN:CD	1:D:780:GLY:HA3	2.39	0.48
1:C:704:ASN:CG	1:C:706:GLN:HG2	2.40	0.47
1:D:752:MET:SD	6:D:479:HOH:O	2.45	0.47
1:C:621:GLU:O	1:C:621:GLU:HG2	2.08	0.47
1:B:553:SER:HB3	1:B:600:LEU:HB3	1.95	0.47
1:B:633:MET:CB	6:B:294:HOH:O	2.61	0.47
1:C:592:ARG:HG2	1:C:647:TYR:HA	1.96	0.47
1:C:803:LEU:O	1:C:804:ASP:HB2	2.15	0.47
1:B:573:ILE:HD13	1:B:624:SER:HB3	1.96	0.47
1:C:557:GLY:N	1:C:578:LYS:NZ	2.63	0.47
1:B:579:LEU:CD1	1:B:581:VAL:HG23	2.45	0.46
1:B:579:LEU:HD13	1:B:581:VAL:CG2	2.45	0.46
1:C:730:VAL:C	1:C:731:LEU:HD12	2.41	0.46
1:A:579:LEU:HD12	1:A:579:LEU:O	2.16	0.46
1:A:612:THR:CB	1:A:616:LEU:HG	2.36	0.46
1:A:573:ILE:CG2	1:A:627:SER:HB2	2.46	0.46
1:C:613:THR:CG2	1:C:614:THR:H	2.07	0.46
1:B:671:ARG:HG3	1:B:688:PHE:HB2	1.97	0.46
1:C:745:TYR:CZ	1:C:750:LYS:HB3	2.51	0.46
1:C:706:GLN:OE1	1:C:706:GLN:CA	2.60	0.45
5:D:1763:ATP:O1B	5:D:1763:ATP:H5'2	2.16	0.45
1:D:743:PHE:CE1	1:D:747:LEU:HD13	2.52	0.45
1:C:659:LEU:CG	1:C:779:LEU:HD21	2.47	0.45
1:C:777:PHE:O	1:C:778:GLY:O	2.35	0.45
1:C:648:LYS:HG3	1:C:649:LYS:HB2	1.98	0.45
5:D:1763:ATP:O1B	5:D:1763:ATP:O1A	2.35	0.45
1:C:613:THR:C	1:C:614:THR:CG2	2.89	0.45
1:D:701:PRO:O	1:D:704:ASN:O	2.34	0.45
1:C:613:THR:N	6:C:430:HOH:O	2.49	0.45
1:D:552:ILE:N	6:D:437:HOH:O	2.50	0.45
1:A:668:MET:HE1	1:A:690:MET:HA	1.99	0.44
1:A:700:SER:HA	1:A:701:PRO:HD3	1.79	0.44
1:A:752:MET:HE2	1:A:752:MET:HB3	1.77	0.44
1:C:649:LYS:N	1:C:653:GLN:HG2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:GLU:O	1:C:578:LYS:HE2	2.14	0.44
1:A:649:LYS:HB2	1:A:649:LYS:HE3	1.68	0.44
1:C:613:THR:O	1:C:614:THR:CG2	2.65	0.44
1:A:727:TYR:CD1	1:A:782:LEU:HD12	2.53	0.44
1:C:731:LEU:N	1:C:731:LEU:CD1	2.80	0.44
1:B:579:LEU:HD12	1:B:579:LEU:C	2.43	0.43
1:B:752:MET:CE	1:B:769:ILE:HD13	2.48	0.43
1:C:749:ASN:C	1:C:750:LYS:HG2	2.43	0.43
1:C:593:GLU:OE2	1:C:649:LYS:CE	2.58	0.43
5:C:1762:ATP:O2B	5:C:1762:ATP:O3G	2.35	0.43
1:B:807:VAL:HG23	6:B:423:HOH:O	2.18	0.43
5:B:1761:ATP:O1A	5:B:1761:ATP:O1B	2.36	0.43
1:D:686:ILE:HD11	1:D:740:PHE:CD1	2.53	0.43
1:A:762:ASP:OD1	1:A:764:TYR:OH	2.27	0.43
1:C:659:LEU:HD13	1:C:779:LEU:HD22	1.97	0.43
1:C:752:MET:HE3	1:C:752:MET:HB2	1.96	0.43
1:B:621:GLU:CD	1:B:621:GLU:N	2.75	0.43
1:A:579:LEU:C	1:A:579:LEU:CD1	2.89	0.43
1:C:659:LEU:HD21	1:C:779:LEU:CD2	2.45	0.43
1:B:574:ARG:NE	1:B:610:LEU:HD13	2.34	0.43
1:B:614:THR:CG2	1:B:615:LYS:N	2.66	0.43
1:B:762:ASP:N	6:B:249:HOH:O	2.05	0.43
1:C:630:ASN:OD1	1:C:633:MET:HG2	2.19	0.42
1:A:796:CYS:HB2	1:A:800:CYS:HB2	2.01	0.42
1:A:807:VAL:HG13	6:A:442:HOH:O	2.18	0.42
1:D:668:MET:HE3	1:D:691:SER:O	2.19	0.42
1:A:579:LEU:CG	6:A:238:HOH:O	2.61	0.42
1:D:552:ILE:O	1:D:553:SER:HB2	2.20	0.42
1:D:611:GLY:HA2	1:D:612:THR:HA	1.72	0.42
1:C:581:VAL:HG12	6:C:94:HOH:O	2.20	0.41
1:C:736:THR:HB	1:C:737:PRO:HD3	2.03	0.41
1:D:762:ASP:HB2	6:D:356:HOH:O	2.19	0.41
1:B:555:GLU:HG3	1:B:556:THR:N	2.35	0.41
1:B:736:THR:N	1:B:737:PRO:CD	2.82	0.41
1:C:654:GLN:O	1:C:654:GLN:HG2	2.20	0.41
1:D:647:TYR:CE1	1:D:659:LEU:HD21	2.54	0.41
1:C:745:TYR:CE1	1:C:750:LYS:HB3	2.55	0.41
1:D:706:GLN:HA	1:D:707:PRO:HD2	1.92	0.41
1:C:574:ARG:NE	1:C:610:LEU:HD11	2.35	0.41
1:C:745:TYR:CZ	1:C:750:LYS:HD2	2.56	0.41
1:A:727:TYR:HD1	1:A:782:LEU:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:THR:OG1	1:C:606:GLU:HG2	2.21	0.41
1:D:671:ARG:NH2	1:D:690:MET:HE2	2.36	0.41
1:B:555:GLU:HG3	1:B:556:THR:H	1.86	0.40
1:D:766:ALA:N	1:D:767:PRO:CD	2.85	0.40
1:A:617:PHE:CD2	1:A:617:PHE:C	2.99	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)
1:A:615:LYS:NZ	1:B:801:ALA:CB[4_554]	1.09	1.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	238/307 (78%)	231 (97%)	5 (2%)	2 (1%)	16	16
1	B	248/307 (81%)	238 (96%)	7 (3%)	3 (1%)	10	8
1	C	241/307 (78%)	231 (96%)	9 (4%)	1 (0%)	30	34
1	D	249/307 (81%)	233 (94%)	12 (5%)	4 (2%)	7	6
All	All	976/1228 (80%)	933 (96%)	33 (3%)	10 (1%)	12	11

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	702	SER
1	D	611	GLY
1	D	704	ASN
1	D	649	LYS
1	A	655	ALA

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Mol	Chain	Res	Type
1	B	701	PRO
1	C	778	GLY
1	B	704	ASN
1	D	702	SER
1	A	611	GLY

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	217/269 (81%)	215 (99%)	2 (1%)	70	84
1	B	225/269 (84%)	219 (97%)	6 (3%)	39	53
1	C	221/269 (82%)	215 (97%)	6 (3%)	39	53
1	D	225/269 (84%)	219 (97%)	6 (3%)	39	53
All	All	888/1076 (82%)	868 (98%)	20 (2%)	44	59

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	579	LEU
1	A	621	GLU
1	B	552	ILE
1	B	613	THR
1	B	620	ILE
1	B	621	GLU
1	B	641	LYS
1	B	809	LEU
1	C	555	GLU
1	C	621	GLU
1	C	648	LYS
1	C	653	GLN
1	C	731	LEU
1	C	779	LEU
1	D	555	GLU
1	D	614	THR

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Mol	Chain	Res	Type
1	D	637	LYS
1	D	650	GLU
1	D	747	LEU
1	D	768	GLN

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

Mol	Chain	Res	Type
1	A	638	ASN
1	A	733	ASN
1	A	758	GLN
1	B	607	ASN
1	B	629	ASN
1	B	630	ASN
1	B	638	ASN
1	B	770	HIS
1	C	607	ASN
1	C	638	ASN
1	C	733	ASN
1	C	770	HIS
1	D	607	ASN
1	D	638	ASN
1	D	679	GLN
1	D	723	ASN
1	D	758	GLN
1	D	768	GLN
1	D	770	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

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	PO4	C	5957	-	4,4,4	0.86	0	6,6,6	0.68	0
5	ATP	D	1763	4	32,33,33	1.44	5 (15%)	48,52,52	1.85	12 (25%)
2	PO4	D	5958	-	4,4,4	1.00	0	6,6,6	0.66	0
2	PO4	D	5960	-	4,4,4	0.94	0	6,6,6	0.49	0
5	ATP	B	1761	4	32,33,33	1.42	6 (18%)	48,52,52	1.89	13 (27%)
2	PO4	A	5955	-	4,4,4	0.94	0	6,6,6	0.78	0
5	ATP	A	1760	4	32,33,33	1.52	6 (18%)	48,52,52	1.65	10 (20%)
2	PO4	B	5959	-	4,4,4	0.94	0	6,6,6	0.47	0
2	PO4	B	5956	-	4,4,4	1.05	0	6,6,6	0.68	0
5	ATP	C	1762	4	32,33,33	1.45	6 (18%)	48,52,52	1.87	11 (22%)

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
5	ATP	A	1760	4	-	1/22/38/38	0/3/3/3
5	ATP	C	1762	4	-	1/22/38/38	0/3/3/3
5	ATP	D	1763	4	-	2/22/38/38	0/3/3/3
5	ATP	B	1761	4	-	2/22/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1760	ATP	C5-C4	4.74	1.47	1.39
5	C	1762	ATP	C5-C4	4.68	1.47	1.39
5	B	1761	ATP	C5-C4	4.36	1.46	1.39
5	D	1763	ATP	C5-C4	4.14	1.46	1.39
5	D	1763	ATP	PB-O3A	4.04	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1761	ATP	PB-O3A	3.60	1.63	1.59
5	A	1760	ATP	PB-O3A	3.53	1.63	1.59
5	C	1762	ATP	PB-O3A	3.24	1.63	1.59
5	A	1760	ATP	C5-C6	2.66	1.48	1.41
5	D	1763	ATP	C4-N9	-2.66	1.32	1.37
5	B	1761	ATP	C8-N7	2.59	1.36	1.31
5	C	1762	ATP	C5-N7	-2.56	1.34	1.39
5	C	1762	ATP	C5-C6	2.49	1.47	1.41
5	C	1762	ATP	C8-N7	2.49	1.36	1.31
5	A	1760	ATP	C8-N7	2.39	1.36	1.31
5	B	1761	ATP	C4-N9	-2.33	1.32	1.37
5	B	1761	ATP	C5-C6	2.31	1.47	1.41
5	D	1763	ATP	C5-C6	2.30	1.47	1.41
5	A	1760	ATP	C4-N9	-2.25	1.33	1.37
5	C	1762	ATP	C4-N9	-2.22	1.33	1.37
5	A	1760	ATP	C5-N7	-2.18	1.35	1.39
5	B	1761	ATP	C5-N7	-2.16	1.35	1.39
5	D	1763	ATP	C5-N7	-2.00	1.35	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1762	ATP	C5-C4-N3	-5.53	119.10	126.72
5	A	1760	ATP	C5-C4-N3	-5.15	119.62	126.72
5	B	1761	ATP	C5-C4-N3	-5.09	119.71	126.72
5	C	1762	ATP	O3A-PA-O1A	-4.79	96.30	110.70
5	D	1763	ATP	C5-C4-N3	-4.62	120.35	126.72
5	C	1762	ATP	N3-C4-N9	4.60	134.99	127.17
5	B	1761	ATP	N3-C4-N9	4.35	134.57	127.17
5	B	1761	ATP	N3-C2-N1	-4.25	122.14	128.58
5	A	1760	ATP	N3-C4-N9	4.17	134.26	127.17
5	D	1763	ATP	N3-C4-N9	4.16	134.25	127.17
5	D	1763	ATP	N3-C2-N1	-4.05	122.44	128.58
5	B	1761	ATP	C4-N9-C8	3.90	109.83	105.74
5	B	1761	ATP	C2-N3-C4	3.87	121.27	111.83
5	D	1763	ATP	C4-N9-C8	3.86	109.79	105.74
5	D	1763	ATP	O3A-PA-O1A	-3.82	99.20	110.70
5	A	1760	ATP	N3-C2-N1	-3.73	122.94	128.58
5	C	1762	ATP	C2-N3-C4	3.71	120.90	111.83
5	A	1760	ATP	C2-N3-C4	3.66	120.78	111.83
5	C	1762	ATP	N3-C2-N1	-3.61	123.11	128.58
5	D	1763	ATP	C2-N3-C4	3.49	120.36	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1763	ATP	O2A-PA-O3A	3.21	115.94	107.27
5	B	1761	ATP	O3A-PA-O1A	-3.12	101.33	110.70
5	B	1761	ATP	C4-C5-N7	-3.06	107.08	110.58
5	A	1760	ATP	C4-C5-N7	-3.00	107.15	110.58
5	C	1762	ATP	C4-N9-C8	2.99	108.87	105.74
5	C	1762	ATP	C4-C5-N7	-2.91	107.25	110.58
5	A	1760	ATP	C4-N9-C8	2.88	108.77	105.74
5	B	1761	ATP	N9-C8-N7	-2.71	110.09	113.94
5	B	1761	ATP	O2A-PA-O3A	2.70	114.58	107.27
5	D	1763	ATP	C4-C5-N7	-2.67	107.53	110.58
5	D	1763	ATP	C2-N1-C6	2.65	123.09	118.73
5	C	1762	ATP	O2A-PA-O3A	2.45	113.89	107.27
5	B	1761	ATP	C5-N7-C8	2.44	107.28	103.45
5	B	1761	ATP	C2-N1-C6	2.43	122.72	118.73
5	B	1761	ATP	C6-C5-N7	2.42	136.76	132.09
5	D	1763	ATP	N9-C8-N7	-2.36	110.58	113.94
5	A	1760	ATP	C2-N1-C6	2.34	122.57	118.73
5	C	1762	ATP	C5-N7-C8	2.21	106.92	103.45
5	A	1760	ATP	C5-N7-C8	2.21	106.92	103.45
5	A	1760	ATP	C6-C5-N7	2.16	136.25	132.09
5	D	1763	ATP	C6-C5-N7	2.11	136.15	132.09
5	C	1762	ATP	C2-N1-C6	2.09	122.17	118.73
5	D	1763	ATP	C5-N7-C8	2.06	106.69	103.45
5	B	1761	ATP	O3G-PG-O2G	2.04	115.46	107.80
5	C	1762	ATP	N9-C8-N7	-2.04	111.04	113.94
5	A	1760	ATP	N9-C8-N7	-2.03	111.06	113.94

There are no chirality outliers.

All (6) torsion outliers are listed below:

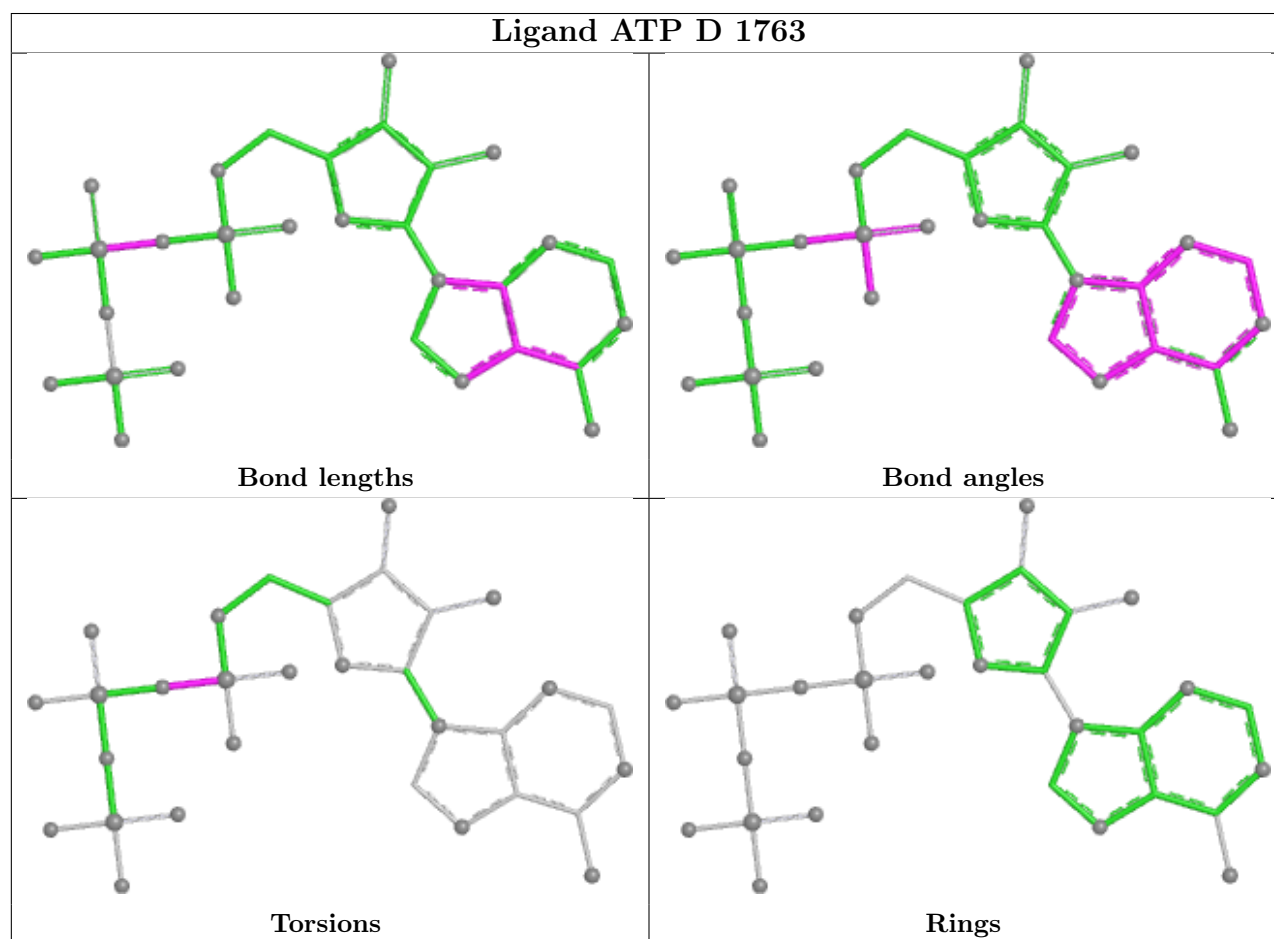
Mol	Chain	Res	Type	Atoms
5	B	1761	ATP	PB-O3B-PG-O2G
5	B	1761	ATP	PB-O3B-PG-O3G
5	D	1763	ATP	PB-O3A-PA-O1A
5	A	1760	ATP	PB-O3B-PG-O1G
5	C	1762	ATP	PB-O3A-PA-O2A
5	D	1763	ATP	PB-O3A-PA-O2A

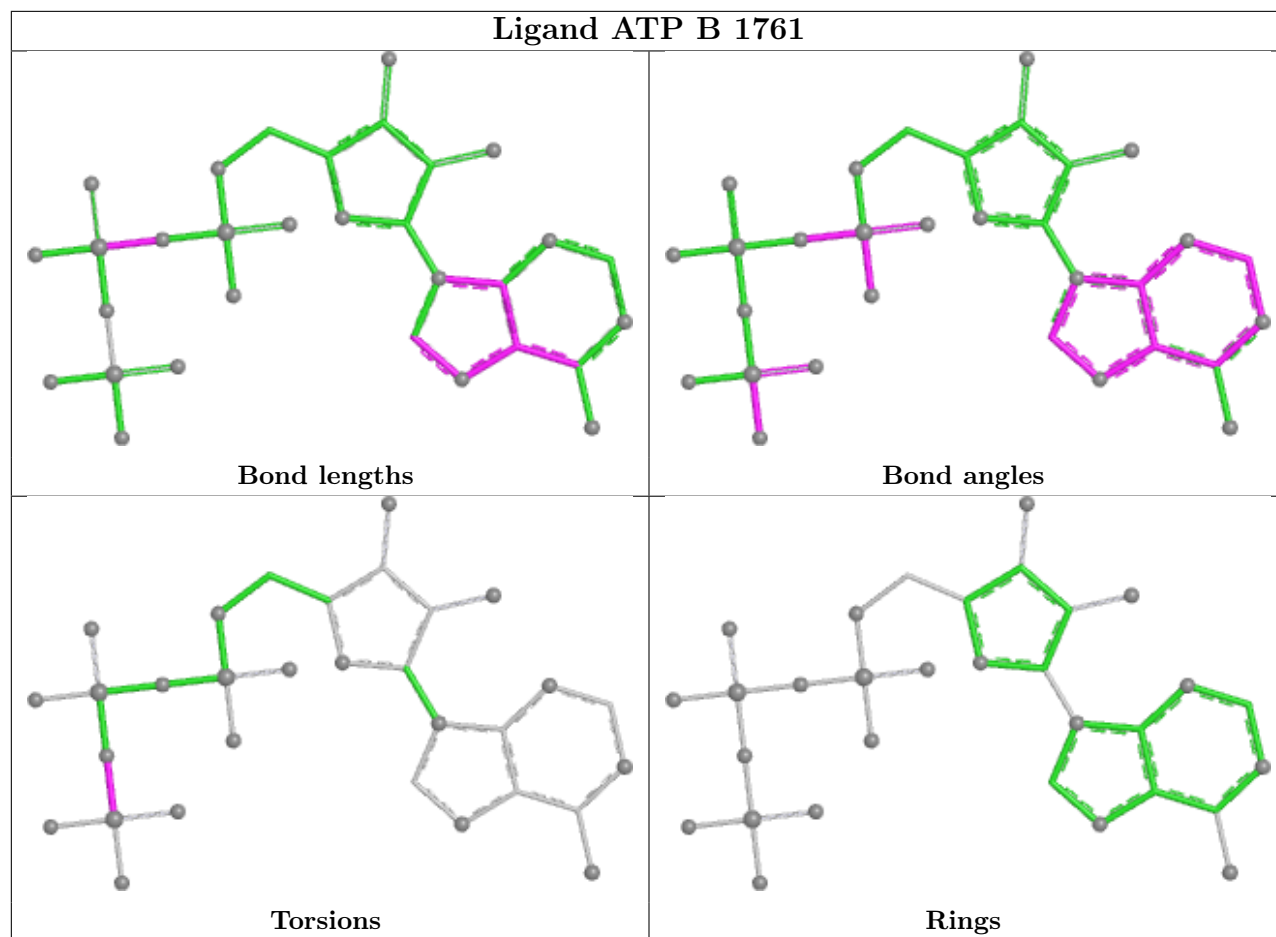
There are no ring outliers.

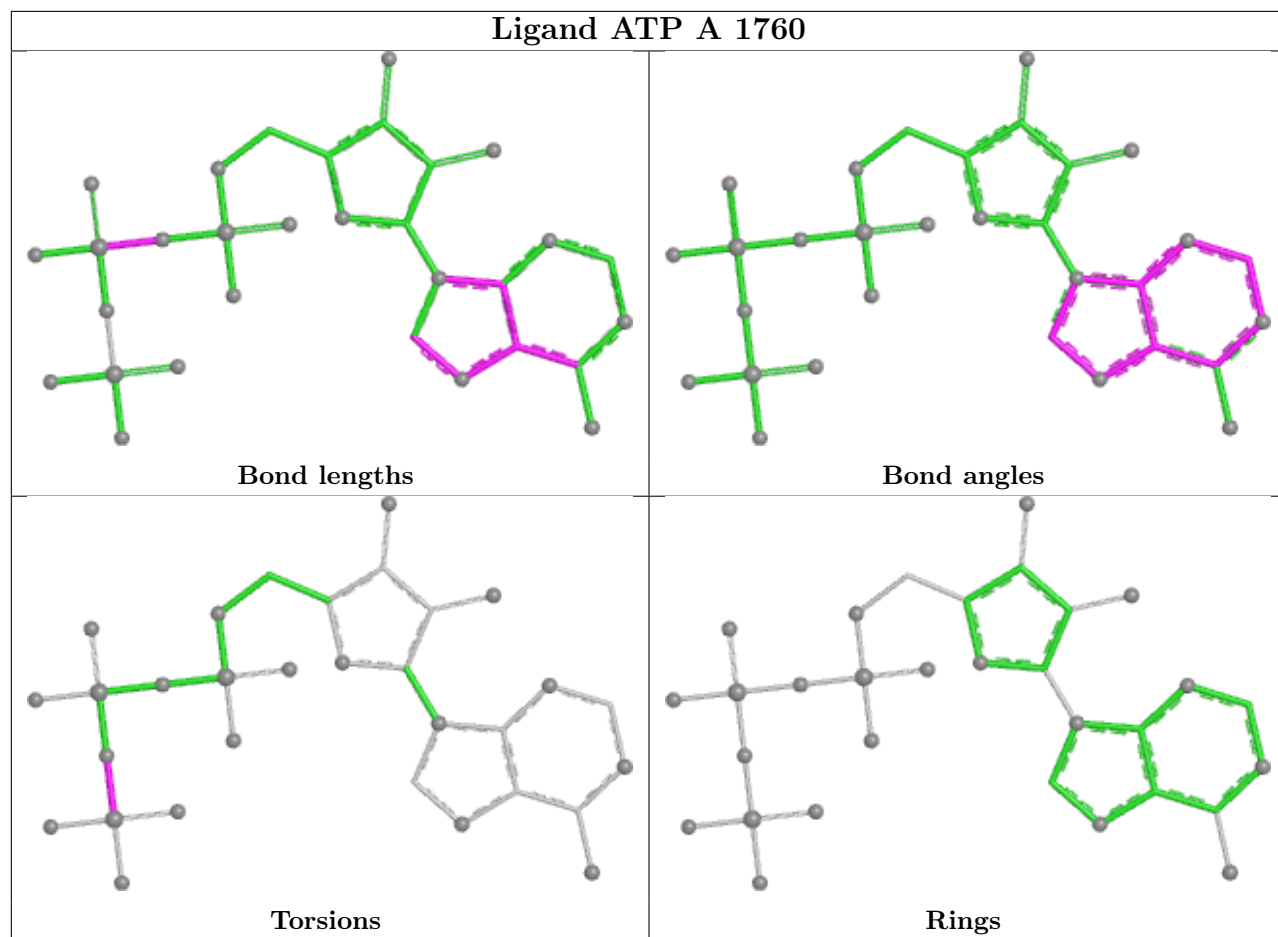
5 monomers are involved in 9 short contacts:

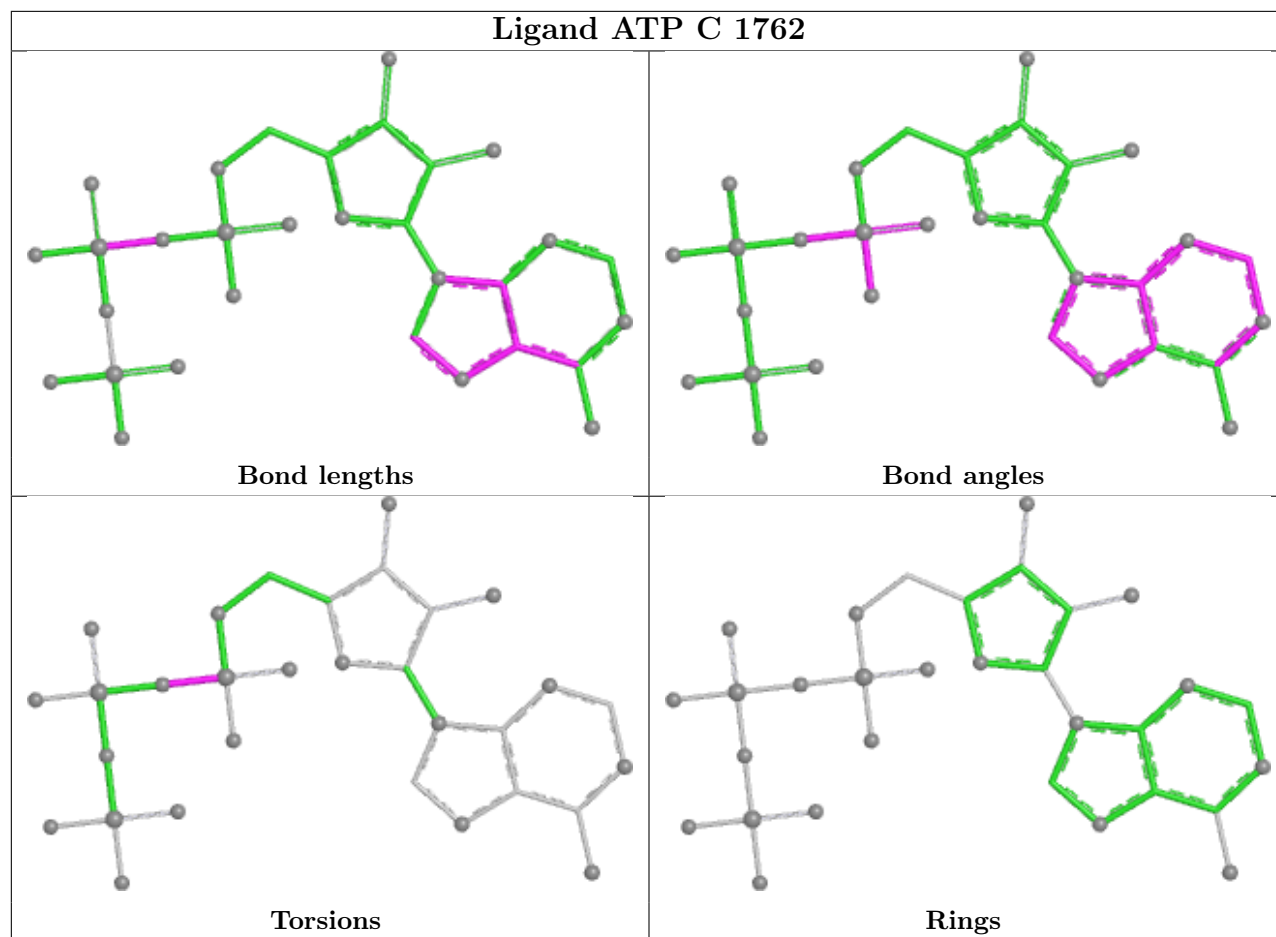
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1763	ATP	3	0
2	D	5960	PO4	1	0
5	B	1761	ATP	2	0
2	B	5959	PO4	1	0
5	C	1762	ATP	2	0

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	246/307 (80%)	-1.55	0 100 100	9, 20, 40, 50	0
1	B	254/307 (82%)	-1.57	0 100 100	6, 16, 43, 55	0
1	C	250/307 (81%)	-1.53	0 100 100	9, 20, 42, 57	0
1	D	253/307 (82%)	-1.57	0 100 100	7, 16, 42, 50	0
All	All	1003/1228 (81%)	-1.55	0 100 100	6, 18, 42, 57	0

There are no RSRZ outliers to report.

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 oligosaccharides 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. 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.

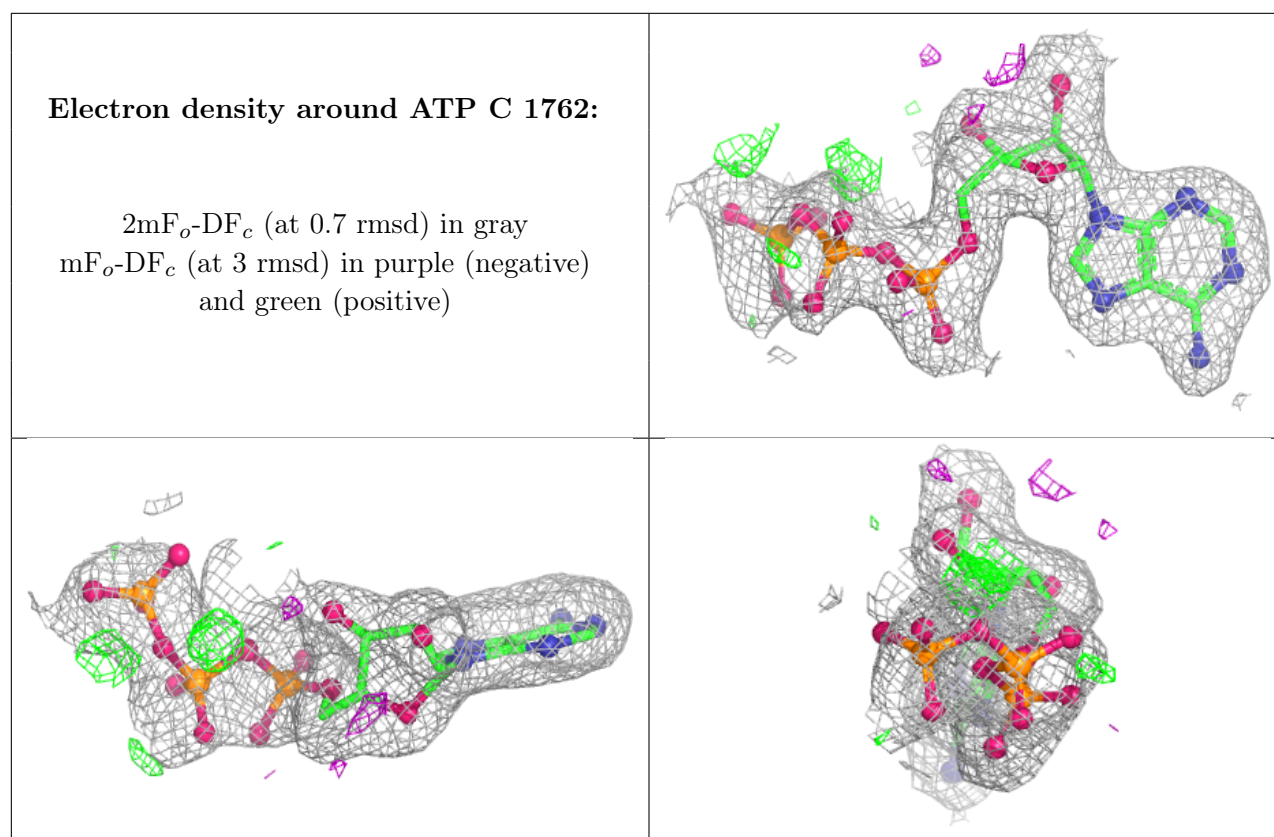
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	B	5959	5/5	0.99	0.05	89,89,89,89	0
2	PO4	D	5960	5/5	0.99	0.05	87,87,87,87	0
4	MG	A	1006	1/1	0.99	0.01	21,21,21,21	0
4	MG	B	1005	1/1	0.99	0.03	22,22,22,22	0

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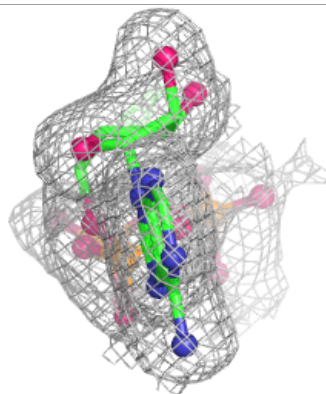
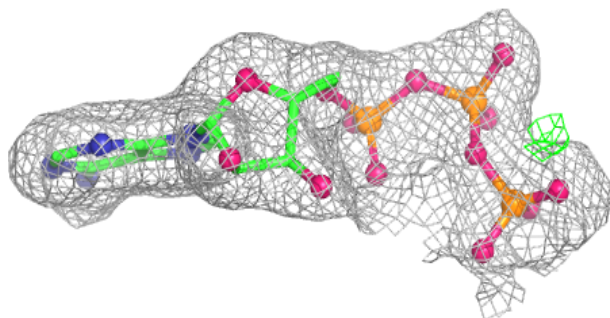
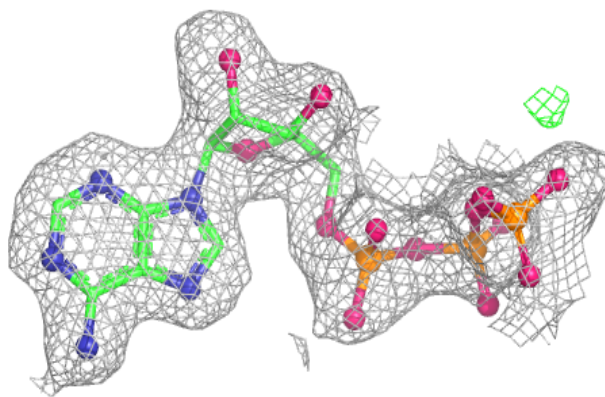
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	C	1007	1/1	0.99	0.02	24,24,24,24	0
4	MG	D	1008	1/1	0.99	0.01	21,21,21,21	0
5	ATP	C	1762	31/31	0.99	0.03	12,16,41,42	0
3	ZN	B	1002	1/1	1.00	0.00	13,13,13,13	0
3	ZN	C	1003	1/1	1.00	0.01	18,18,18,18	0
3	ZN	D	1004	1/1	1.00	0.01	14,14,14,14	0
2	PO4	A	5955	5/5	1.00	0.01	14,17,18,19	0
2	PO4	C	5957	5/5	1.00	0.02	18,19,20,20	0
2	PO4	D	5958	5/5	1.00	0.02	20,21,22,23	0
2	PO4	B	5956	5/5	1.00	0.02	17,18,19,20	0
5	ATP	A	1760	31/31	1.00	0.02	9,19,42,43	0
5	ATP	B	1761	31/31	1.00	0.02	7,16,42,43	0
3	ZN	A	1001	1/1	1.00	0.01	17,17,17,17	0
5	ATP	D	1763	31/31	1.00	0.03	8,17,43,44	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.

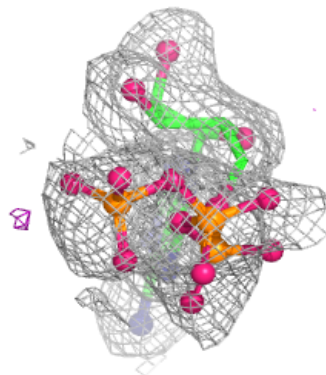
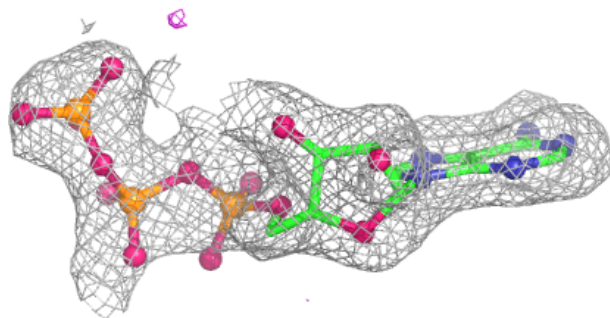
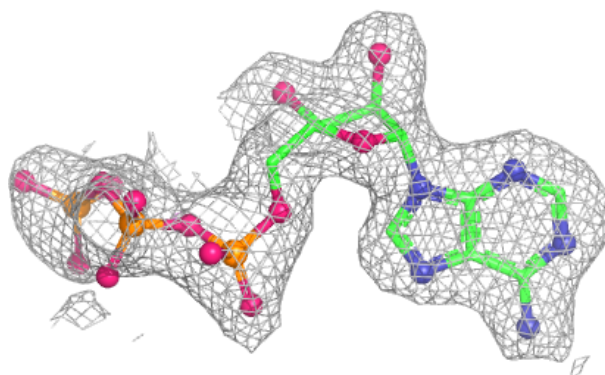


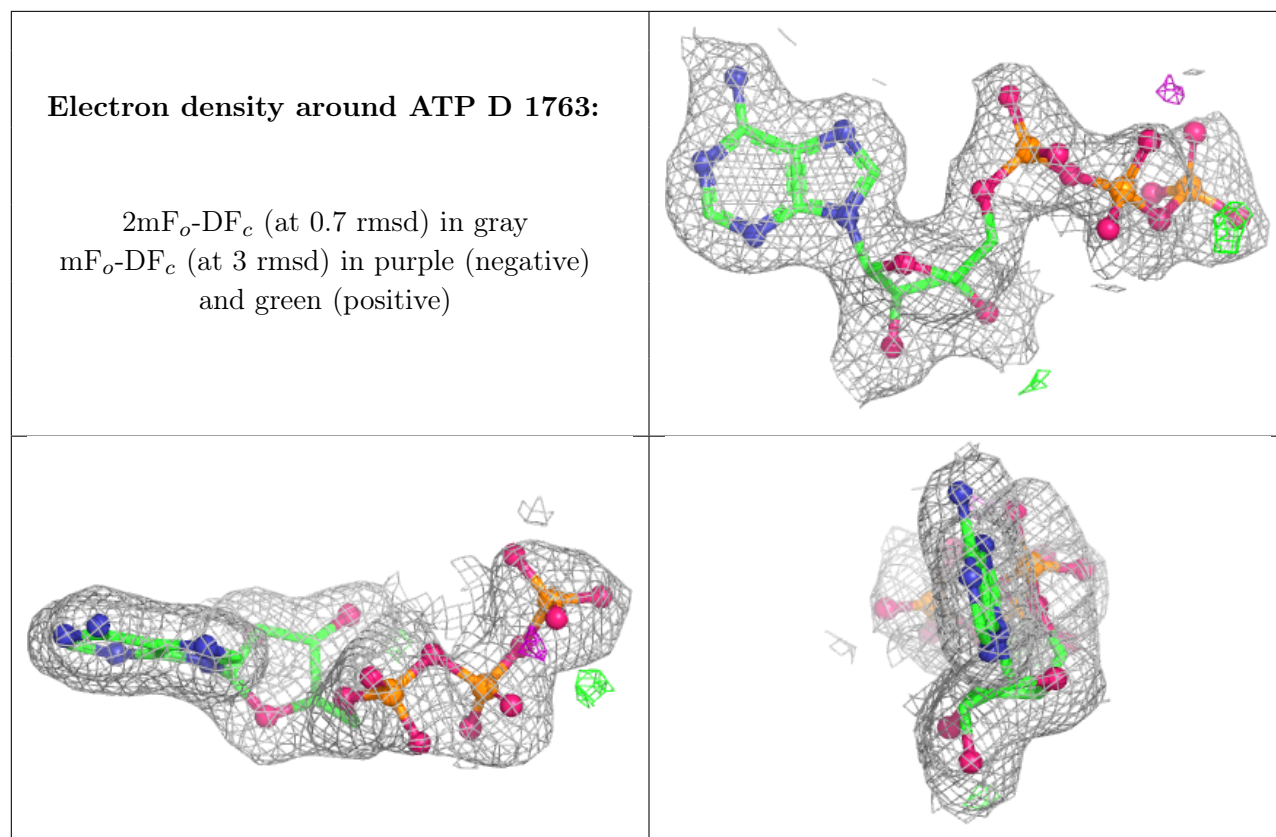
Electron density around ATP A 1760:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ATP B 1761:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.