



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:33 am BST

PDB ID : 3QB0  
Title : Crystal structure of Actin-related protein Arp4 from *S. cerevisiae* complexed with ATP  
Authors : Fenn, S.; Breitsprecher, D.; Gerhold, C.B.; Witte, G.; Faix, J.; Hopfner, K.P.  
Deposited on : 2011-01-12  
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

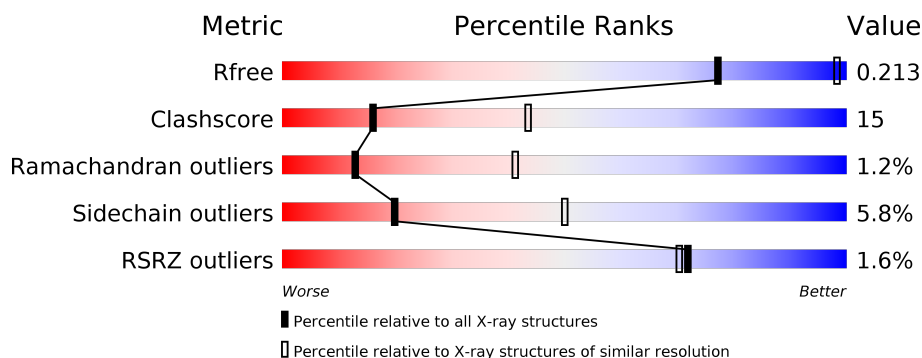
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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	498	<div> <div>2%</div> <div> <div>61%</div> <div>21%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	498	<div> <div>%</div> <div> <div>58%</div> <div>25%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	498	<div> <div>%</div> <div> <div>58%</div> <div>25%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	498	<div> <div>%</div> <div> <div>60%</div> <div>23%</div> <div>•</div> <div>14%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13785 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 Actin-related protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	134	0	0
			3396	2161	568	656	11			
1	B	430	Total	C	N	O	S	111	0	0
			3420	2178	571	660	11			
1	C	430	Total	C	N	O	S	111	0	0
			3421	2177	572	661	11			
1	D	430	Total	C	N	O	S	105	0	0
			3420	2175	572	662	11			

There are 36 discrepancies between the modelled and reference sequences:

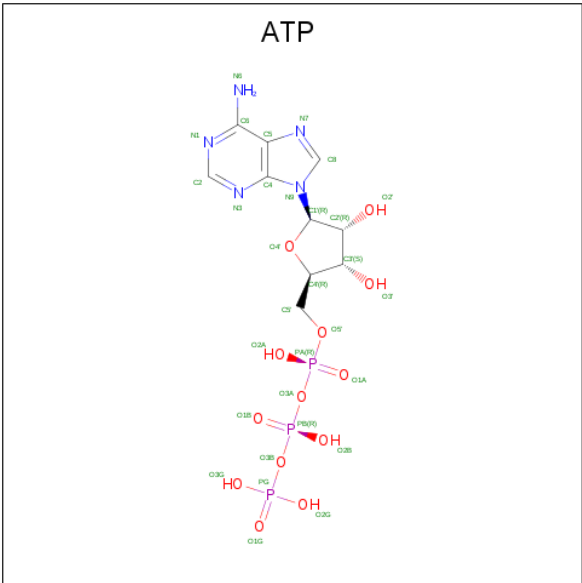
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	UNP P80428
A	-7	LYS	-	EXPRESSION TAG	UNP P80428
A	-6	HIS	-	EXPRESSION TAG	UNP P80428
A	-5	HIS	-	EXPRESSION TAG	UNP P80428
A	-4	HIS	-	EXPRESSION TAG	UNP P80428
A	-3	HIS	-	EXPRESSION TAG	UNP P80428
A	-2	HIS	-	EXPRESSION TAG	UNP P80428
A	-1	HIS	-	EXPRESSION TAG	UNP P80428
A	0	LYS	-	EXPRESSION TAG	UNP P80428
B	-8	MET	-	EXPRESSION TAG	UNP P80428
B	-7	LYS	-	EXPRESSION TAG	UNP P80428
B	-6	HIS	-	EXPRESSION TAG	UNP P80428
B	-5	HIS	-	EXPRESSION TAG	UNP P80428
B	-4	HIS	-	EXPRESSION TAG	UNP P80428
B	-3	HIS	-	EXPRESSION TAG	UNP P80428
B	-2	HIS	-	EXPRESSION TAG	UNP P80428
B	-1	HIS	-	EXPRESSION TAG	UNP P80428
B	0	LYS	-	EXPRESSION TAG	UNP P80428
C	-8	MET	-	EXPRESSION TAG	UNP P80428
C	-7	LYS	-	EXPRESSION TAG	UNP P80428
C	-6	HIS	-	EXPRESSION TAG	UNP P80428

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	EXPRESSION TAG	UNP P80428
C	-4	HIS	-	EXPRESSION TAG	UNP P80428
C	-3	HIS	-	EXPRESSION TAG	UNP P80428
C	-2	HIS	-	EXPRESSION TAG	UNP P80428
C	-1	HIS	-	EXPRESSION TAG	UNP P80428
C	0	LYS	-	EXPRESSION TAG	UNP P80428
D	-8	MET	-	EXPRESSION TAG	UNP P80428
D	-7	LYS	-	EXPRESSION TAG	UNP P80428
D	-6	HIS	-	EXPRESSION TAG	UNP P80428
D	-5	HIS	-	EXPRESSION TAG	UNP P80428
D	-4	HIS	-	EXPRESSION TAG	UNP P80428
D	-3	HIS	-	EXPRESSION TAG	UNP P80428
D	-2	HIS	-	EXPRESSION TAG	UNP P80428
D	-1	HIS	-	EXPRESSION TAG	UNP P80428
D	0	LYS	-	EXPRESSION TAG	UNP P80428

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

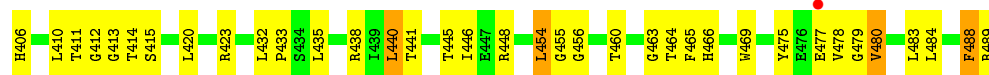
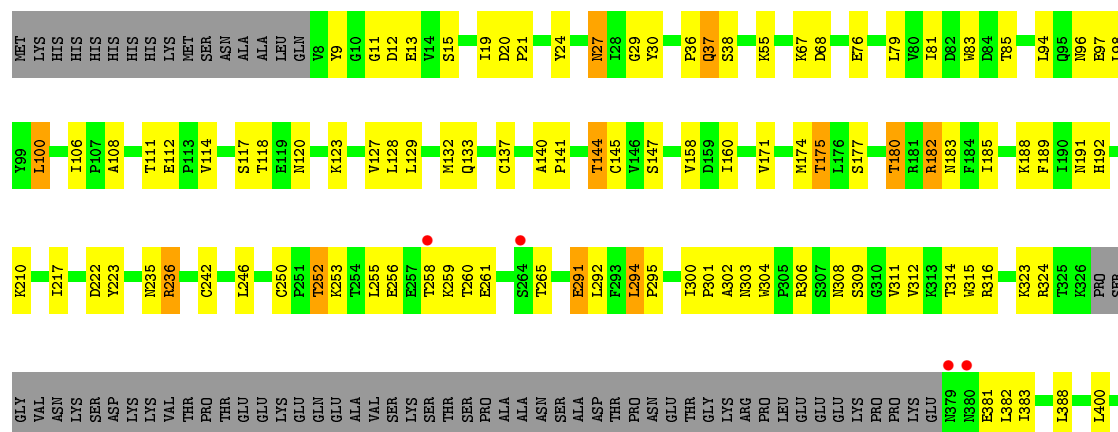
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

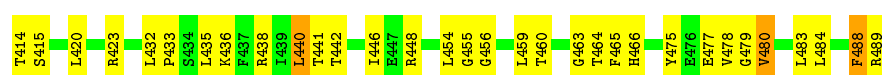
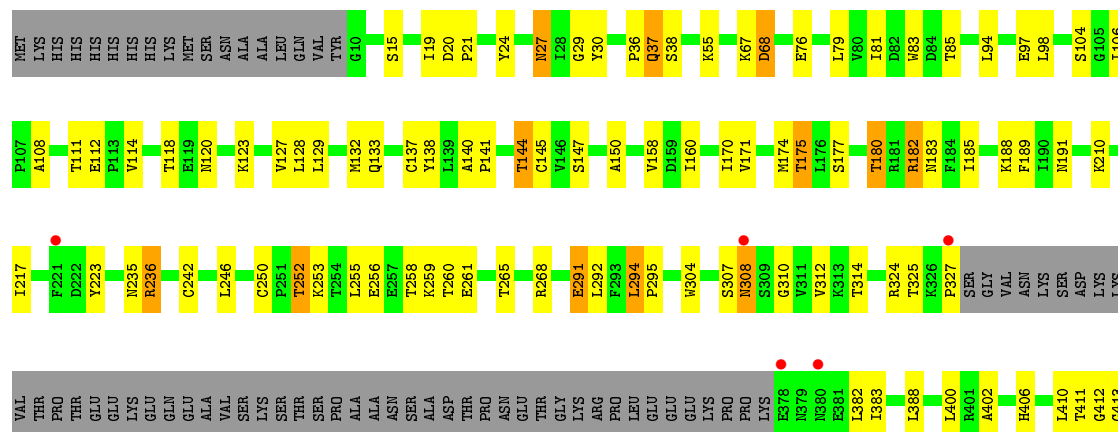




• Molecule 1: Actin-related protein 4



• Molecule 1: Actin-related protein 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.81Å 118.81Å 395.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.54 – 3.40 49.54 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.54-3.40) 99.9 (49.54-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.192 , 0.221 0.186 , 0.213	Depositor DCC
$R_{free}$ test set	2118 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.7	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 63.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.084 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13785	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 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.24	0/3471	0.44	0/4707
1	B	0.24	0/3497	0.45	1/4744 (0.0%)
1	C	0.24	0/3497	0.47	2/4743 (0.0%)
1	D	0.24	0/3496	0.44	0/4742
All	All	0.24	0/13961	0.45	3/18936 (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	C	440	LEU	CB-CG-CD1	5.83	120.91	111.00
1	C	100	LEU	CB-CG-CD2	5.80	120.85	111.00
1	B	483	LEU	CB-CG-CD1	5.54	120.42	111.00

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	3396	0	3363	94	0
1	B	3420	0	3381	104	0
1	C	3421	0	3380	100	0
1	D	3420	0	3382	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	0	12	2	0
2	B	31	0	12	2	0
2	C	31	0	12	2	0
2	D	31	0	12	2	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
All	All	13785	0	13554	380	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (380) 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:30:TYR:H	1:A:37:GLN:HE21	1.20	0.87
1:D:30:TYR:H	1:D:37:GLN:HE21	1.21	0.86
1:B:30:TYR:H	1:B:37:GLN:HE21	1.20	0.85
1:C:30:TYR:H	1:C:37:GLN:HE21	1.21	0.85
1:A:191:ASN:HD22	1:A:235:ASN:HD22	1.24	0.84
1:B:191:ASN:HD22	1:B:235:ASN:HD22	1.25	0.84
1:D:191:ASN:HD22	1:D:235:ASN:HD22	1.24	0.82
1:C:478:VAL:HG23	1:C:480:VAL:HG12	1.62	0.82
1:C:191:ASN:HD22	1:C:235:ASN:HD22	1.24	0.81
1:D:55:LYS:NZ	1:D:85:THR:HG22	1.96	0.80
1:B:189:PHE:HE2	1:B:291:GLU:HG2	1.46	0.80
1:A:55:LYS:NZ	1:A:85:THR:HG22	1.97	0.79
1:C:55:LYS:NZ	1:C:85:THR:HG22	1.98	0.79
1:A:478:VAL:HG23	1:A:480:VAL:HG12	1.63	0.79
1:B:55:LYS:NZ	1:B:85:THR:HG22	1.98	0.78
1:A:189:PHE:HE2	1:A:291:GLU:HG2	1.47	0.78
1:C:189:PHE:HE2	1:C:291:GLU:HG2	1.47	0.78
1:D:189:PHE:HE2	1:D:291:GLU:HG2	1.47	0.77
1:D:413:GLY:HA3	2:D:490:ATP:H5'1	1.67	0.77
1:B:413:GLY:HA3	2:B:490:ATP:H5'1	1.65	0.77
1:C:413:GLY:HA3	2:C:490:ATP:H5'1	1.65	0.77
1:A:291:GLU:HG3	1:A:295:PRO:HA	1.69	0.74
1:B:478:VAL:CG1	1:B:480:VAL:HG12	2.17	0.73
1:D:478:VAL:CG1	1:D:480:VAL:HG12	2.18	0.73
1:D:291:GLU:HG3	1:D:295:PRO:HA	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:HE2	1:A:255:LEU:HB2	1.73	0.71
1:C:291:GLU:HG3	1:C:295:PRO:HA	1.72	0.71
1:B:182:ARG:CZ	1:B:312:VAL:HG12	2.21	0.70
1:C:478:VAL:CG2	1:C:480:VAL:HG12	2.21	0.70
1:C:182:ARG:CZ	1:C:312:VAL:HG12	2.21	0.70
1:B:291:GLU:HG3	1:B:295:PRO:HA	1.72	0.69
1:A:478:VAL:CG2	1:A:480:VAL:HG12	2.23	0.69
1:A:34:ASP:OD2	1:B:213:LYS:HD2	1.95	0.66
1:D:150:ALA:HA	1:D:442:THR:HG21	1.77	0.66
1:B:9:TYR:HB3	1:D:402:ALA:CB	2.26	0.65
1:A:413:GLY:HA3	2:A:490:ATP:H5'1	1.78	0.64
1:A:446:ILE:CD1	1:B:210:LYS:HG3	2.28	0.64
1:C:210:LYS:HG3	1:D:446:ILE:HD11	1.77	0.64
1:A:446:ILE:HD11	1:B:210:LYS:HG3	1.80	0.64
1:C:480:VAL:HG22	1:C:483:LEU:H	1.64	0.62
1:A:480:VAL:HG22	1:A:483:LEU:H	1.65	0.62
1:A:150:ALA:HA	1:A:442:THR:HG21	1.80	0.62
1:D:480:VAL:HG22	1:D:483:LEU:H	1.65	0.62
1:D:325:THR:O	1:D:327:PRO:HD3	1.99	0.61
1:B:480:VAL:HG22	1:B:483:LEU:H	1.65	0.61
1:A:171:VAL:HG21	1:A:400:LEU:HD13	1.82	0.60
1:B:144:THR:O	1:B:147:SER:HB3	2.02	0.60
1:B:309:SER:OG	1:B:311:VAL:HG22	2.02	0.60
1:C:55:LYS:HZ1	1:C:85:THR:HG22	1.67	0.60
1:C:210:LYS:HG3	1:D:446:ILE:CD1	2.32	0.59
1:D:141:PRO:HB2	1:D:144:THR:HG22	1.84	0.59
1:D:144:THR:O	1:D:147:SER:HB3	2.03	0.59
1:A:144:THR:O	1:A:147:SER:HB3	2.02	0.59
1:B:141:PRO:HB2	1:B:144:THR:HG22	1.85	0.58
1:C:191:ASN:ND2	1:C:235:ASN:HD22	1.99	0.58
1:C:309:SER:OG	1:C:311:VAL:HG22	2.02	0.58
1:A:141:PRO:HB2	1:A:144:THR:HG22	1.84	0.58
1:C:141:PRO:HB2	1:C:144:THR:HG22	1.84	0.58
1:A:34:ASP:CG	1:B:213:LYS:HD2	2.24	0.58
1:C:441:THR:HG21	1:C:448:ARG:HH22	1.69	0.58
1:A:415:SER:HA	1:A:420:LEU:HD23	1.86	0.58
1:D:83:TRP:HE1	1:D:120:ASN:ND2	2.02	0.58
1:A:191:ASN:HD22	1:A:235:ASN:ND2	2.00	0.57
1:C:415:SER:HA	1:C:420:LEU:HD23	1.86	0.57
1:A:83:TRP:HE1	1:A:120:ASN:ND2	2.02	0.57
1:C:191:ASN:HD22	1:C:235:ASN:ND2	2.00	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:THR:O	1:C:147:SER:HB3	2.03	0.57
1:D:415:SER:HA	1:D:420:LEU:HD23	1.87	0.57
1:B:191:ASN:ND2	1:B:235:ASN:HD22	2.00	0.57
1:C:475:TYR:O	1:C:479:GLY:HA2	2.06	0.56
1:B:441:THR:HG21	1:B:448:ARG:HH22	1.70	0.56
1:C:189:PHE:CE1	1:C:300:ILE:HG12	2.40	0.56
1:C:189:PHE:CE2	1:C:291:GLU:HG2	2.36	0.56
1:D:478:VAL:HG12	1:D:480:VAL:H	1.71	0.56
1:C:83:TRP:HE1	1:C:120:ASN:ND2	2.03	0.56
1:D:55:LYS:HZ3	1:D:85:THR:HG22	1.69	0.56
1:B:83:TRP:HE1	1:B:120:ASN:ND2	2.03	0.56
1:B:415:SER:HA	1:B:420:LEU:HD23	1.86	0.55
1:B:478:VAL:HG12	1:B:480:VAL:H	1.71	0.55
1:B:171:VAL:HG21	1:B:400:LEU:HD13	1.87	0.55
1:B:191:ASN:HD22	1:B:235:ASN:ND2	2.01	0.55
1:D:475:TYR:O	1:D:479:GLY:HA2	2.06	0.55
1:B:183:ASN:ND2	1:B:388:LEU:HD22	2.21	0.55
1:B:478:VAL:HG12	1:B:480:VAL:HG12	1.88	0.55
1:B:475:TYR:O	1:B:479:GLY:HA2	2.05	0.55
1:A:35:PHE:CE2	1:B:214:PRO:HD3	2.42	0.55
1:D:191:ASN:HD22	1:D:235:ASN:ND2	2.00	0.55
1:B:9:TYR:HB3	1:D:402:ALA:HB3	1.87	0.55
1:C:183:ASN:ND2	1:C:388:LEU:HD22	2.21	0.55
1:A:459:LEU:HB3	1:A:465:PHE:CE2	2.42	0.55
1:D:55:LYS:HZ1	1:D:85:THR:HG22	1.72	0.55
1:D:189:PHE:CE2	1:D:291:GLU:HG2	2.37	0.54
1:D:171:VAL:HG21	1:D:400:LEU:HD13	1.88	0.54
1:A:144:THR:HB	1:A:175:THR:HG22	1.90	0.54
1:A:183:ASN:ND2	1:A:388:LEU:HD22	2.23	0.54
1:B:67:LYS:HB2	1:B:223:TYR:CG	2.43	0.54
1:D:459:LEU:HB3	1:D:465:PHE:CE2	2.42	0.54
1:B:189:PHE:CE1	1:B:300:ILE:HG12	2.42	0.54
1:C:114:VAL:HG11	1:C:180:THR:HG21	1.90	0.54
1:C:188:LYS:HE2	1:C:304:TRP:CZ2	2.43	0.54
1:C:171:VAL:HG21	1:C:400:LEU:HD13	1.90	0.54
1:A:189:PHE:CE2	1:A:291:GLU:HG2	2.36	0.54
1:B:188:LYS:HE2	1:B:304:TRP:CZ2	2.43	0.54
1:C:250:CYS:HB2	1:C:252:THR:O	2.08	0.54
1:A:475:TYR:O	1:A:479:GLY:HA2	2.07	0.54
1:D:478:VAL:HG12	1:D:480:VAL:HG12	1.88	0.53
1:C:11:GLY:C	1:C:13:GLU:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HZ1	1:A:85:THR:HG22	1.70	0.53
1:B:11:GLY:C	1:B:13:GLU:H	2.12	0.53
1:B:189:PHE:CE2	1:B:291:GLU:HG2	2.36	0.53
1:C:413:GLY:CA	2:C:490:ATP:H5'1	2.37	0.53
1:A:480:VAL:HG13	1:A:480:VAL:O	2.08	0.53
1:B:55:LYS:HZ1	1:B:85:THR:HG22	1.73	0.53
1:B:480:VAL:HG13	1:B:480:VAL:O	2.09	0.53
1:C:24:TYR:CZ	1:C:236:ARG:NH1	2.77	0.53
1:D:261:GLU:O	1:D:265:THR:HB	2.08	0.53
1:A:67:LYS:HB2	1:A:223:TYR:CG	2.44	0.53
1:B:24:TYR:CZ	1:B:236:ARG:NH1	2.77	0.53
1:C:144:THR:HB	1:C:175:THR:HG22	1.91	0.53
1:C:480:VAL:O	1:C:480:VAL:HG13	2.09	0.53
1:B:114:VAL:HG11	1:B:180:THR:HG21	1.90	0.52
1:B:185:ILE:HG22	1:B:292:LEU:HD23	1.91	0.52
1:A:114:VAL:HG11	1:A:180:THR:HG21	1.91	0.52
1:A:261:GLU:O	1:A:265:THR:HB	2.09	0.52
1:C:67:LYS:HB2	1:C:223:TYR:CG	2.43	0.52
1:B:144:THR:HB	1:B:175:THR:HG22	1.91	0.52
1:B:250:CYS:HB2	1:B:252:THR:O	2.08	0.52
1:D:114:VAL:HG11	1:D:180:THR:HG21	1.91	0.52
1:D:67:LYS:HB2	1:D:223:TYR:CG	2.44	0.52
1:D:144:THR:HB	1:D:175:THR:HG22	1.91	0.52
1:A:250:CYS:HB2	1:A:252:THR:O	2.09	0.52
1:C:185:ILE:HG22	1:C:292:LEU:HD23	1.92	0.52
1:B:446:ILE:HD12	1:B:446:ILE:N	2.25	0.52
1:B:261:GLU:O	1:B:265:THR:HB	2.09	0.52
1:B:294:LEU:H	1:B:294:LEU:HD22	1.74	0.52
1:B:413:GLY:CA	2:B:490:ATP:H5'1	2.39	0.52
1:D:191:ASN:ND2	1:D:235:ASN:HD22	1.99	0.52
1:B:55:LYS:HZ3	1:B:85:THR:HG22	1.71	0.52
1:D:480:VAL:O	1:D:480:VAL:HG13	2.09	0.52
1:B:411:THR:HG22	1:B:412:GLY:H	1.75	0.51
1:C:67:LYS:HB2	1:C:223:TYR:CD2	2.45	0.51
1:D:185:ILE:HG22	1:D:292:LEU:HD23	1.93	0.51
1:A:24:TYR:CZ	1:A:236:ARG:NH1	2.78	0.51
1:A:83:TRP:HE1	1:A:120:ASN:HD22	1.59	0.51
1:D:250:CYS:HB2	1:D:252:THR:O	2.09	0.51
1:C:38:SER:HB2	1:C:97:GLU:HB2	1.92	0.51
1:D:24:TYR:CZ	1:D:236:ARG:NH1	2.79	0.51
1:A:185:ILE:HG22	1:A:292:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LYS:HB2	1:A:223:TYR:CD2	2.46	0.51
1:C:128:LEU:HD23	1:C:132:MET:HE1	1.91	0.51
1:C:446:ILE:HD12	1:C:446:ILE:N	2.25	0.51
1:A:191:ASN:ND2	1:A:235:ASN:HD22	1.99	0.51
1:C:261:GLU:O	1:C:265:THR:HB	2.09	0.51
1:B:325:THR:O	1:B:327:PRO:HD3	2.11	0.51
1:D:446:ILE:N	1:D:446:ILE:HD12	2.25	0.51
1:C:411:THR:HG22	1:C:412:GLY:H	1.76	0.51
1:C:250:CYS:O	1:C:423:ARG:HD3	2.10	0.51
1:A:38:SER:HB2	1:A:97:GLU:HB2	1.92	0.50
1:B:67:LYS:HB2	1:B:223:TYR:CD2	2.46	0.50
1:B:38:SER:HB2	1:B:97:GLU:HB2	1.92	0.50
1:A:37:GLN:HG3	1:A:98:LEU:HD13	1.93	0.50
1:A:55:LYS:HZ3	1:A:85:THR:HG22	1.73	0.50
1:B:83:TRP:HE1	1:B:120:ASN:HD22	1.59	0.50
1:B:406:HIS:CE1	1:B:438:ARG:HD3	2.46	0.50
1:D:83:TRP:HE1	1:D:120:ASN:HD22	1.58	0.50
1:D:37:GLN:HG3	1:D:98:LEU:HD13	1.93	0.50
1:D:128:LEU:HD23	1:D:132:MET:HE1	1.93	0.50
1:D:67:LYS:HB2	1:D:223:TYR:CD2	2.46	0.50
1:D:294:LEU:HD22	1:D:294:LEU:H	1.76	0.50
1:D:183:ASN:ND2	1:D:388:LEU:HD22	2.26	0.50
1:D:38:SER:HB2	1:D:97:GLU:HB2	1.92	0.50
1:B:9:TYR:HB3	1:D:402:ALA:HB1	1.92	0.50
1:D:441:THR:HG21	1:D:448:ARG:HH22	1.77	0.50
1:A:446:ILE:HD12	1:A:446:ILE:N	2.26	0.50
1:D:411:THR:HG22	1:D:412:GLY:H	1.76	0.50
1:A:294:LEU:H	1:A:294:LEU:HD22	1.76	0.49
1:A:406:HIS:CE1	1:A:438:ARG:HD3	2.48	0.49
1:A:411:THR:HG22	1:A:412:GLY:H	1.77	0.49
1:B:128:LEU:HD23	1:B:132:MET:HE1	1.92	0.49
1:D:158:VAL:HB	1:D:410:LEU:HD23	1.94	0.49
1:C:294:LEU:HD22	1:C:294:LEU:H	1.76	0.49
1:C:83:TRP:HE1	1:C:120:ASN:HD22	1.59	0.49
1:B:250:CYS:O	1:B:423:ARG:HD3	2.12	0.49
1:B:37:GLN:HG3	1:B:98:LEU:HD13	1.94	0.49
1:C:406:HIS:CE1	1:C:438:ARG:HD3	2.47	0.49
1:A:441:THR:HG21	1:A:448:ARG:HH22	1.78	0.49
1:C:112:GLU:O	1:C:141:PRO:HA	2.13	0.49
1:C:55:LYS:HZ3	1:C:85:THR:HG22	1.77	0.49
1:D:123:LYS:O	1:D:127:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:HIS:CE1	1:D:438:ARG:HD3	2.48	0.48
1:B:158:VAL:HB	1:B:410:LEU:HD23	1.95	0.48
1:B:438:ARG:HG2	1:B:440:LEU:HD21	1.95	0.48
1:B:9:TYR:HD2	1:B:11:GLY:H	1.61	0.48
1:A:258:THR:HG23	1:A:259:LYS:N	2.29	0.48
1:A:112:GLU:O	1:A:141:PRO:HA	2.13	0.48
1:C:9:TYR:HD2	1:C:11:GLY:H	1.61	0.48
1:D:112:GLU:O	1:D:141:PRO:HA	2.14	0.48
1:D:258:THR:HG23	1:D:259:LYS:N	2.29	0.48
1:B:112:GLU:O	1:B:141:PRO:HA	2.13	0.47
1:A:123:LYS:O	1:A:127:VAL:HG23	2.13	0.47
1:B:258:THR:HG23	1:B:259:LYS:N	2.29	0.47
1:B:300:ILE:HD12	1:B:382:LEU:HD21	1.95	0.47
1:C:37:GLN:HG3	1:C:98:LEU:HD13	1.94	0.47
1:D:438:ARG:HG2	1:D:440:LEU:HD21	1.96	0.47
1:D:294:LEU:HD22	1:D:294:LEU:N	2.30	0.47
1:A:294:LEU:N	1:A:294:LEU:HD22	2.30	0.47
1:B:294:LEU:N	1:B:294:LEU:HD22	2.29	0.47
1:C:158:VAL:HB	1:C:410:LEU:HD23	1.97	0.47
1:D:111:THR:HA	1:D:140:ALA:O	2.15	0.47
1:B:488:PHE:O	1:B:489:ARG:HB2	2.15	0.47
1:C:258:THR:HG23	1:C:259:LYS:N	2.30	0.47
1:D:242:CYS:O	1:D:246:LEU:HB2	2.15	0.47
1:B:242:CYS:O	1:B:246:LEU:HB2	2.14	0.47
1:B:302:ALA:O	1:B:303:ASN:ND2	2.48	0.47
1:D:463:GLY:O	1:D:466:HIS:HB2	2.15	0.47
1:A:242:CYS:O	1:A:246:LEU:HB2	2.15	0.47
1:C:106:ILE:N	1:C:106:ILE:HD12	2.30	0.47
1:C:177:SER:CB	1:C:314:THR:HG21	2.45	0.47
1:B:19:ILE:HG22	1:B:21:PRO:HD3	1.97	0.47
1:C:111:THR:HA	1:C:140:ALA:O	2.15	0.47
1:C:242:CYS:O	1:C:246:LEU:HB2	2.15	0.47
1:C:294:LEU:HD22	1:C:294:LEU:N	2.30	0.47
1:A:463:GLY:O	1:A:466:HIS:HB2	2.15	0.46
1:C:160:ILE:HG22	1:C:414:THR:HB	1.97	0.46
1:B:411:THR:HG22	1:B:412:GLY:N	2.31	0.46
1:B:441:THR:HG21	1:B:448:ARG:NH2	2.30	0.46
1:C:123:LYS:O	1:C:127:VAL:HG23	2.15	0.46
1:C:177:SER:HB3	1:C:314:THR:HG21	1.96	0.46
1:D:106:ILE:N	1:D:106:ILE:HD12	2.31	0.46
1:D:488:PHE:O	1:D:489:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:HB	1:A:410:LEU:HD23	1.97	0.46
1:A:488:PHE:O	1:A:489:ARG:HB2	2.15	0.46
1:B:160:ILE:HG22	1:B:414:THR:HB	1.98	0.46
1:B:117:SER:HA	1:B:315:TRP:CE3	2.51	0.46
1:C:19:ILE:HG22	1:C:21:PRO:HD3	1.97	0.46
1:B:123:LYS:O	1:B:127:VAL:HG23	2.14	0.46
1:C:300:ILE:HD12	1:C:382:LEU:HD21	1.98	0.46
1:C:441:THR:HG21	1:C:448:ARG:NH2	2.30	0.46
1:B:76:GLU:HB2	1:B:81:ILE:HD13	1.97	0.46
1:C:171:VAL:HG13	1:C:324:ARG:HH22	1.81	0.46
1:A:127:VAL:HG12	1:A:132:MET:HE2	1.98	0.46
1:A:111:THR:HA	1:A:140:ALA:O	2.15	0.46
1:B:253:LYS:HG2	1:B:255:LEU:H	1.81	0.46
1:B:177:SER:CB	1:B:314:THR:HG21	2.46	0.46
1:D:411:THR:HG22	1:D:412:GLY:N	2.31	0.46
1:B:106:ILE:HD12	1:B:106:ILE:N	2.30	0.45
1:C:302:ALA:O	1:C:303:ASN:ND2	2.49	0.45
1:C:117:SER:HA	1:C:315:TRP:CE3	2.50	0.45
1:C:76:GLU:HB2	1:C:81:ILE:HD13	1.98	0.45
1:A:438:ARG:HG2	1:A:440:LEU:HD21	1.96	0.45
1:C:253:LYS:HG2	1:C:255:LEU:H	1.80	0.45
1:A:19:ILE:HG22	1:A:21:PRO:HD3	1.99	0.45
1:C:171:VAL:HG13	1:C:324:ARG:NH2	2.31	0.45
1:A:106:ILE:N	1:A:106:ILE:HD12	2.31	0.45
1:B:111:THR:HA	1:B:140:ALA:O	2.15	0.45
1:C:488:PHE:O	1:C:489:ARG:HB2	2.16	0.45
1:B:177:SER:HB3	1:B:314:THR:HG21	1.98	0.45
1:A:227:LYS:HG3	1:A:228:SER:N	2.32	0.45
1:A:76:GLU:HB2	1:A:81:ILE:HD13	1.98	0.45
1:B:177:SER:O	1:B:180:THR:HG23	2.16	0.45
1:D:410:LEU:HB2	1:D:441:THR:HG22	1.98	0.45
1:D:19:ILE:HG22	1:D:21:PRO:HD3	1.98	0.45
1:D:253:LYS:HG2	1:D:255:LEU:H	1.80	0.45
1:B:67:LYS:HA	1:B:68:ASP:HA	1.48	0.45
1:C:177:SER:O	1:C:180:THR:HG23	2.16	0.45
1:A:411:THR:HG22	1:A:412:GLY:N	2.31	0.45
1:D:413:GLY:CA	2:D:490:ATP:H5'1	2.41	0.45
1:A:253:LYS:HG2	1:A:255:LEU:H	1.81	0.44
1:D:383:ILE:HG21	1:D:388:LEU:HD13	1.99	0.44
1:C:411:THR:HG22	1:C:412:GLY:N	2.31	0.44
1:A:383:ILE:HG21	1:A:388:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:LEU:HB2	1:A:441:THR:HG22	1.99	0.44
1:A:129:LEU:O	1:A:133:GLN:HA	2.17	0.44
1:B:129:LEU:O	1:B:133:GLN:HA	2.18	0.44
1:D:177:SER:O	1:D:180:THR:HG23	2.17	0.44
1:D:138:TYR:CE2	1:D:465:PHE:CZ	3.06	0.44
1:B:171:VAL:HG13	1:B:324:ARG:NH2	2.32	0.44
1:B:316:ARG:HD3	1:B:489:ARG:HD3	1.99	0.44
1:D:129:LEU:O	1:D:133:GLN:HA	2.17	0.44
1:C:129:LEU:O	1:C:133:GLN:HA	2.18	0.44
1:A:177:SER:O	1:A:180:THR:HG23	2.18	0.44
1:D:76:GLU:HB2	1:D:81:ILE:HD13	1.99	0.43
1:C:29:GLY:HA2	1:C:37:GLN:HG2	2.01	0.43
1:B:106:ILE:HA	1:B:107:PRO:HD3	1.83	0.43
1:A:128:LEU:HD23	1:A:132:MET:HE1	2.00	0.43
1:A:182:ARG:CZ	1:A:312:VAL:HG12	2.49	0.43
1:C:9:TYR:HD2	1:C:11:GLY:N	2.16	0.43
1:C:96:ASN:OD1	1:D:436:LYS:HD2	2.19	0.43
1:D:67:LYS:HA	1:D:68:ASP:HA	1.48	0.43
1:B:171:VAL:HG13	1:B:324:ARG:HH22	1.82	0.43
1:A:250:CYS:O	1:A:423:ARG:HD3	2.19	0.43
1:B:29:GLY:HA2	1:B:37:GLN:HG2	2.01	0.43
1:B:302:ALA:C	1:B:304:TRP:H	2.22	0.43
1:B:383:ILE:HG21	1:B:388:LEU:HD13	2.01	0.43
1:D:182:ARG:CZ	1:D:312:VAL:HG12	2.49	0.43
1:D:307:SER:O	1:D:308:ASN:C	2.57	0.43
1:B:9:TYR:HD2	1:B:11:GLY:N	2.16	0.43
1:C:454:LEU:HD13	1:C:454:LEU:HA	1.80	0.43
1:A:67:LYS:HA	1:A:68:ASP:HA	1.48	0.43
1:D:188:LYS:HG2	1:D:304:TRP:HH2	1.84	0.43
1:B:94:LEU:HA	1:B:98:LEU:HB2	2.01	0.43
1:C:302:ALA:C	1:C:304:TRP:H	2.22	0.43
1:A:29:GLY:HA2	1:A:37:GLN:HG2	2.00	0.42
1:C:145:CYS:O	1:C:455:GLY:HA3	2.19	0.42
1:A:20:ASP:HA	1:A:111:THR:OG1	2.19	0.42
1:B:192:HIS:NE2	1:B:301:PRO:HG3	2.35	0.42
1:B:463:GLY:O	1:B:466:HIS:HB2	2.18	0.42
1:C:463:GLY:O	1:C:466:HIS:HB2	2.19	0.42
1:D:20:ASP:HA	1:D:111:THR:OG1	2.19	0.42
1:C:383:ILE:HG21	1:C:388:LEU:HD13	2.01	0.42
1:D:160:ILE:HG22	1:D:414:THR:HB	2.02	0.42
1:D:94:LEU:HA	1:D:98:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ASP:HA	1:C:111:THR:OG1	2.20	0.42
1:C:480:VAL:HG13	1:C:484:LEU:HD13	2.02	0.42
1:D:250:CYS:O	1:D:423:ARG:HD3	2.19	0.42
1:C:108:ALA:O	1:C:137:CYS:HA	2.20	0.42
1:C:222:ASP:HB2	1:D:268:ARG:HH12	1.84	0.42
1:C:316:ARG:HD3	1:C:489:ARG:HD3	2.02	0.42
1:C:94:LEU:HA	1:C:98:LEU:HB2	2.02	0.42
1:A:210:LYS:HB3	1:A:217:ILE:O	2.20	0.42
1:A:177:SER:CB	1:A:314:THR:HG21	2.50	0.42
1:A:433:PRO:C	1:A:435:LEU:H	2.23	0.41
1:D:108:ALA:O	1:D:137:CYS:HA	2.20	0.41
1:D:433:PRO:C	1:D:435:LEU:H	2.24	0.41
1:D:145:CYS:O	1:D:455:GLY:HA3	2.20	0.41
1:D:138:TYR:CD2	1:D:465:PHE:CZ	3.08	0.41
1:D:177:SER:CB	1:D:314:THR:HG21	2.51	0.41
1:A:27:ASN:HB3	1:A:36:PRO:HG3	2.02	0.41
1:B:20:ASP:HA	1:B:111:THR:OG1	2.20	0.41
1:B:480:VAL:HG13	1:B:484:LEU:HD13	2.02	0.41
1:D:29:GLY:HA2	1:D:37:GLN:HG2	2.01	0.41
1:A:307:SER:O	1:A:308:ASN:C	2.58	0.41
1:A:177:SER:HB2	1:A:314:THR:HG21	2.02	0.41
1:A:480:VAL:O	1:A:484:LEU:HD13	2.21	0.41
1:C:192:HIS:NE2	1:C:301:PRO:HG3	2.35	0.41
1:C:308:ASN:HB3	1:C:382:LEU:HD12	2.02	0.41
1:A:188:LYS:HG2	1:A:304:TRP:HH2	1.84	0.41
1:D:253:LYS:HB3	1:D:256:GLU:CD	2.41	0.41
1:A:106:ILE:HA	1:A:107:PRO:HD3	1.83	0.41
1:A:480:VAL:HG13	1:A:484:LEU:HD13	2.02	0.41
1:B:145:CYS:O	1:B:455:GLY:HA3	2.20	0.41
1:B:253:LYS:HB3	1:B:256:GLU:CD	2.41	0.41
1:B:27:ASN:HB3	1:B:36:PRO:HG3	2.03	0.41
1:C:210:LYS:HB3	1:C:217:ILE:O	2.21	0.41
1:D:324:ARG:HA	1:D:324:ARG:HD3	1.85	0.41
1:A:253:LYS:HB3	1:A:256:GLU:CD	2.41	0.41
1:D:185:ILE:HD12	1:D:185:ILE:N	2.36	0.41
1:A:138:TYR:CE2	1:A:465:PHE:CZ	3.08	0.41
1:D:27:ASN:HB3	1:D:36:PRO:HG3	2.02	0.41
1:D:456:GLY:O	1:D:460:THR:HG23	2.21	0.41
1:C:27:ASN:HB3	1:C:36:PRO:HG3	2.03	0.41
1:C:480:VAL:O	1:C:484:LEU:HD13	2.21	0.41
1:A:413:GLY:CA	2:A:490:ATP:H5'1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:LEU:HD23	1:C:410:LEU:HA	1.90	0.41
1:D:310:GLY:N	1:D:383:ILE:HD12	2.36	0.41
1:A:138:TYR:CD2	1:A:465:PHE:CZ	3.08	0.41
1:B:108:ALA:O	1:B:137:CYS:HA	2.20	0.41
1:C:294:LEU:HA	1:C:295:PRO:HD3	1.89	0.41
1:C:433:PRO:C	1:C:435:LEU:H	2.24	0.41
1:D:210:LYS:HB3	1:D:217:ILE:O	2.20	0.41
1:D:480:VAL:HG13	1:D:484:LEU:HD13	2.02	0.41
1:D:480:VAL:O	1:D:484:LEU:HD13	2.21	0.41
1:B:121:ARG:O	1:B:124:SER:HB2	2.21	0.40
1:B:225:VAL:HB	1:B:230:TYR:HE2	1.86	0.40
1:A:108:ALA:O	1:A:137:CYS:HA	2.21	0.40
1:A:302:ALA:C	1:A:304:TRP:H	2.25	0.40
1:A:79:LEU:HD12	1:A:79:LEU:H	1.86	0.40
1:B:185:ILE:HD12	1:B:185:ILE:N	2.36	0.40
1:C:253:LYS:HB3	1:C:256:GLU:CD	2.41	0.40
1:C:465:PHE:O	1:C:469:TRP:CD1	2.74	0.40
1:A:185:ILE:HD12	1:A:185:ILE:N	2.36	0.40
1:A:15:SER:HB2	1:C:323:LYS:O	2.22	0.40
1:A:417:ILE:HA	1:A:418:PRO:HD3	1.87	0.40
1:A:94:LEU:HA	1:A:98:LEU:HB2	2.02	0.40
1:B:446:ILE:N	1:B:446:ILE:CD1	2.84	0.40
1:B:480:VAL:O	1:B:484:LEU:HD13	2.21	0.40
1:C:446:ILE:N	1:C:446:ILE:CD1	2.85	0.40
1:B:433:PRO:C	1:B:435:LEU:H	2.24	0.40
1:C:456:GLY:O	1:C:460:THR:HG23	2.21	0.40
1:D:170:ILE:CD1	1:D:175:THR:HB	2.52	0.40

There are no symmetry-related clashes.

## 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	423/498 (85%)	386 (91%)	33 (8%)	4 (1%)	17 49
1	B	426/498 (86%)	383 (90%)	36 (8%)	7 (2%)	9 34
1	C	426/498 (86%)	384 (90%)	37 (9%)	5 (1%)	13 41
1	D	426/498 (86%)	388 (91%)	34 (8%)	4 (1%)	17 49
All	All	1701/1992 (85%)	1541 (91%)	140 (8%)	20 (1%)	13 41

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	THR
1	B	252	THR
1	C	252	THR
1	D	252	THR
1	B	381	GLU
1	B	445	THR
1	C	445	THR
1	B	477	GLU
1	D	477	GLU
1	A	477	GLU
1	B	12	ASP
1	C	12	ASP
1	C	477	GLU
1	D	104	SER
1	A	104	SER
1	B	104	SER
1	A	480	VAL
1	B	480	VAL
1	C	480	VAL
1	D	480	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	380/443 (86%)	359 (94%)	21 (6%)	21 51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	382/443 (86%)	360 (94%)	22 (6%)	20	50
1	C	382/443 (86%)	359 (94%)	23 (6%)	19	49
1	D	383/443 (86%)	361 (94%)	22 (6%)	20	50
All	All	1527/1772 (86%)	1439 (94%)	88 (6%)	20	50

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	27	ASN
1	A	37	GLN
1	A	68	ASP
1	A	79	LEU
1	A	118	THR
1	A	144	THR
1	A	174	MET
1	A	175	THR
1	A	180	THR
1	A	182	ARG
1	A	236	ARG
1	A	260	THR
1	A	291	GLU
1	A	294	LEU
1	A	308	ASN
1	A	432	LEU
1	A	440	LEU
1	A	454	LEU
1	A	464	THR
1	A	488	PHE
1	B	15	SER
1	B	27	ASN
1	B	37	GLN
1	B	68	ASP
1	B	79	LEU
1	B	118	THR
1	B	144	THR
1	B	174	MET
1	B	175	THR
1	B	180	THR
1	B	182	ARG
1	B	236	ARG

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Mol	Chain	Res	Type
1	B	260	THR
1	B	291	GLU
1	B	294	LEU
1	B	306	ARG
1	B	432	LEU
1	B	440	LEU
1	B	454	LEU
1	B	464	THR
1	B	483	LEU
1	B	488	PHE
1	C	15	SER
1	C	27	ASN
1	C	37	GLN
1	C	68	ASP
1	C	79	LEU
1	C	100	LEU
1	C	118	THR
1	C	144	THR
1	C	174	MET
1	C	175	THR
1	C	180	THR
1	C	182	ARG
1	C	236	ARG
1	C	260	THR
1	C	291	GLU
1	C	294	LEU
1	C	306	ARG
1	C	381	GLU
1	C	432	LEU
1	C	440	LEU
1	C	454	LEU
1	C	464	THR
1	C	488	PHE
1	D	15	SER
1	D	27	ASN
1	D	37	GLN
1	D	68	ASP
1	D	79	LEU
1	D	118	THR
1	D	144	THR
1	D	174	MET
1	D	175	THR

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Mol	Chain	Res	Type
1	D	180	THR
1	D	182	ARG
1	D	236	ARG
1	D	260	THR
1	D	291	GLU
1	D	294	LEU
1	D	308	ASN
1	D	382	LEU
1	D	432	LEU
1	D	440	LEU
1	D	454	LEU
1	D	464	THR
1	D	488	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	89	GLN
1	A	120	ASN
1	A	234	ASN
1	A	235	ASN
1	A	240	GLN
1	A	406	HIS
1	B	37	GLN
1	B	89	GLN
1	B	120	ASN
1	B	234	ASN
1	B	235	ASN
1	B	240	GLN
1	B	303	ASN
1	B	406	HIS
1	C	37	GLN
1	C	89	GLN
1	C	120	ASN
1	C	234	ASN
1	C	235	ASN
1	C	240	GLN
1	C	303	ASN
1	C	406	HIS
1	D	37	GLN
1	D	89	GLN

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Mol	Chain	Res	Type
1	D	120	ASN
1	D	234	ASN
1	D	235	ASN
1	D	240	GLN
1	D	406	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	B	490	3	26,33,33	0.92	1 (3%)	31,52,52	1.52	5 (16%)
2	ATP	D	490	3	26,33,33	0.91	1 (3%)	31,52,52	1.51	5 (16%)
2	ATP	A	490	3	26,33,33	0.94	1 (3%)	31,52,52	1.52	6 (19%)
2	ATP	C	490	3	26,33,33	0.92	1 (3%)	31,52,52	1.52	5 (16%)

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	B	490	3	-	5/18/38/38	0/3/3/3
2	ATP	D	490	3	-	5/18/38/38	0/3/3/3
2	ATP	A	490	3	-	5/18/38/38	0/3/3/3
2	ATP	C	490	3	-	6/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	490	ATP	C5-C4	2.52	1.47	1.40
2	B	490	ATP	C5-C4	2.46	1.47	1.40
2	C	490	ATP	C5-C4	2.45	1.47	1.40
2	D	490	ATP	C5-C4	2.43	1.47	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	490	ATP	PB-O3B-PG	-3.17	121.96	132.83
2	C	490	ATP	PA-O3A-PB	-3.08	122.26	132.83
2	A	490	ATP	PB-O3B-PG	-3.07	122.29	132.83
2	B	490	ATP	N3-C2-N1	-3.07	123.88	128.68
2	B	490	ATP	PB-O3B-PG	-3.07	122.31	132.83
2	B	490	ATP	PA-O3A-PB	-3.04	122.39	132.83
2	A	490	ATP	N3-C2-N1	-3.04	123.93	128.68
2	A	490	ATP	PA-O3A-PB	-3.03	122.41	132.83
2	C	490	ATP	N3-C2-N1	-3.03	123.94	128.68
2	C	490	ATP	PB-O3B-PG	-3.02	122.46	132.83
2	D	490	ATP	N3-C2-N1	-3.01	123.97	128.68
2	D	490	ATP	PA-O3A-PB	-2.97	122.63	132.83
2	C	490	ATP	C4-C5-N7	-2.92	106.36	109.40
2	A	490	ATP	C4-C5-N7	-2.84	106.44	109.40
2	D	490	ATP	C4-C5-N7	-2.83	106.45	109.40
2	B	490	ATP	C4-C5-N7	-2.81	106.47	109.40
2	B	490	ATP	C3'-C2'-C1'	2.79	105.18	100.98
2	D	490	ATP	C3'-C2'-C1'	2.79	105.17	100.98
2	C	490	ATP	C3'-C2'-C1'	2.75	105.11	100.98
2	A	490	ATP	C3'-C2'-C1'	2.65	104.97	100.98
2	A	490	ATP	C2'-C3'-C4'	2.04	106.60	102.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

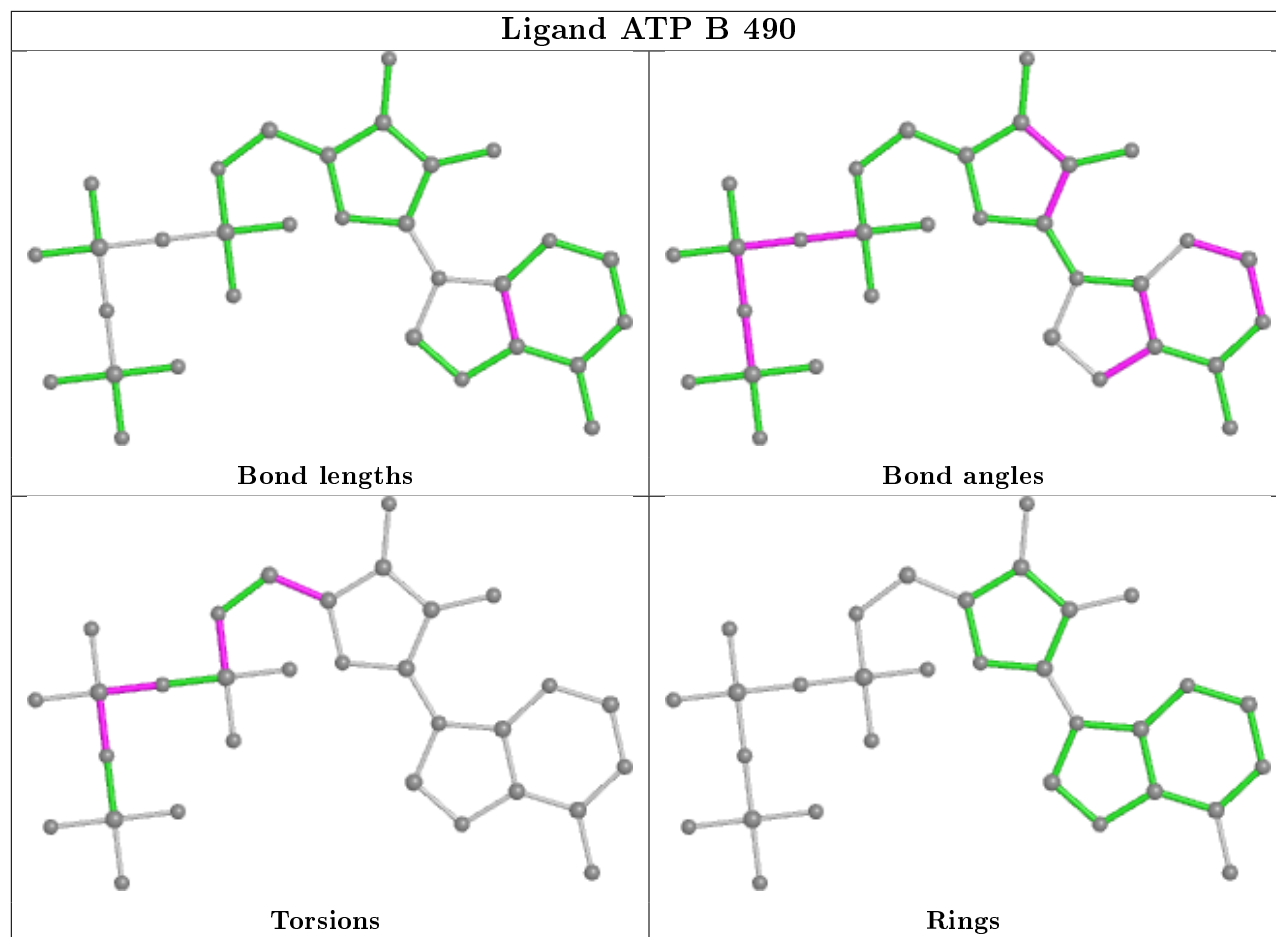
Mol	Chain	Res	Type	Atoms
2	D	490	ATP	C5'-O5'-PA-O3A
2	C	490	ATP	C5'-O5'-PA-O3A
2	B	490	ATP	C5'-O5'-PA-O3A
2	A	490	ATP	C5'-O5'-PA-O3A
2	D	490	ATP	O4'-C4'-C5'-O5'
2	C	490	ATP	O4'-C4'-C5'-O5'
2	B	490	ATP	O4'-C4'-C5'-O5'
2	A	490	ATP	O4'-C4'-C5'-O5'
2	D	490	ATP	C5'-O5'-PA-O1A
2	C	490	ATP	C5'-O5'-PA-O1A
2	B	490	ATP	C5'-O5'-PA-O1A
2	A	490	ATP	C5'-O5'-PA-O1A
2	D	490	ATP	PG-O3B-PB-O2B
2	D	490	ATP	PA-O3A-PB-O1B
2	C	490	ATP	PG-O3B-PB-O2B
2	C	490	ATP	PA-O3A-PB-O1B
2	C	490	ATP	PA-O3A-PB-O2B
2	B	490	ATP	PG-O3B-PB-O2B
2	B	490	ATP	PA-O3A-PB-O1B
2	A	490	ATP	PG-O3B-PB-O2B
2	A	490	ATP	PA-O3A-PB-O1B

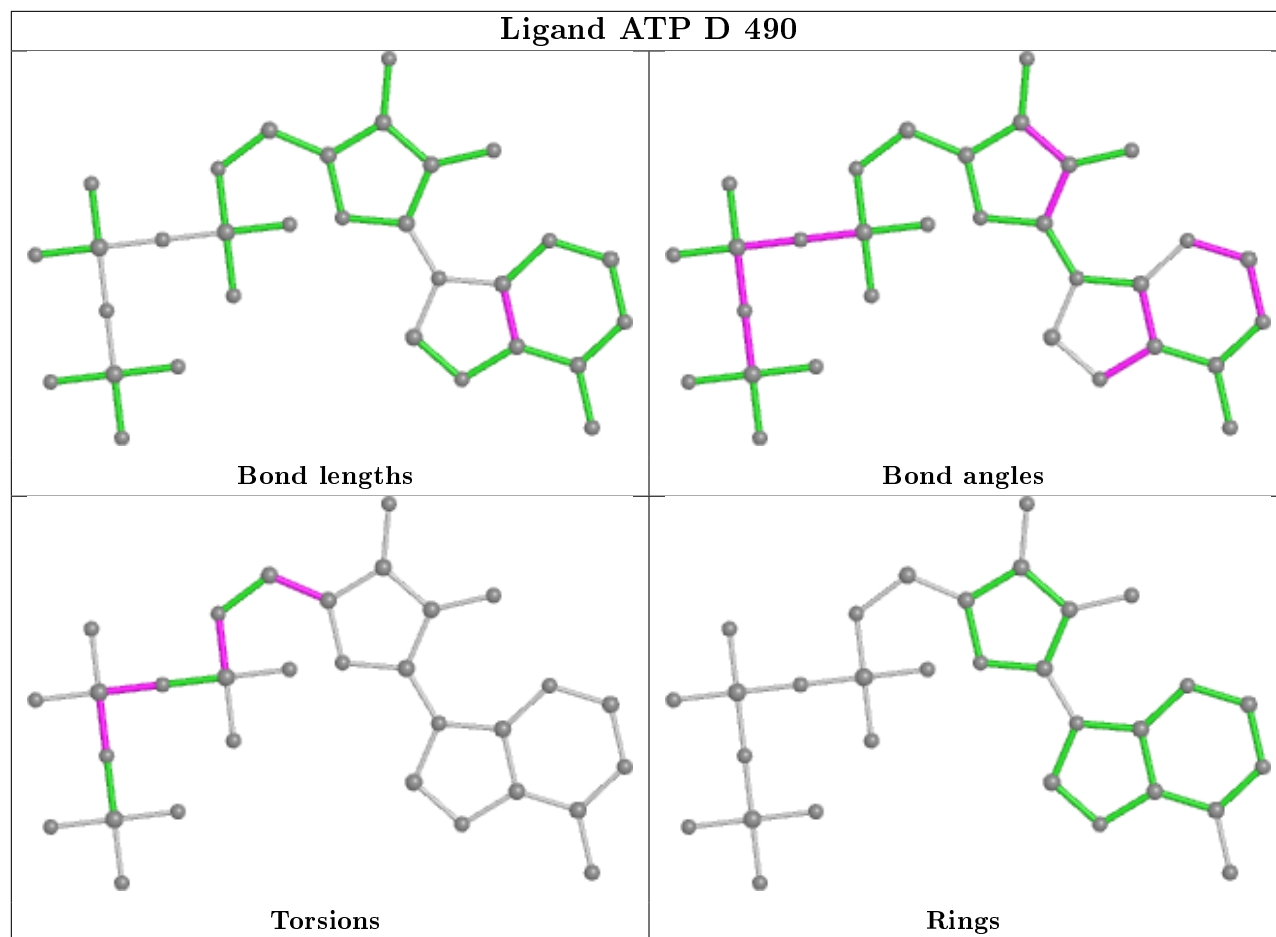
There are no ring outliers.

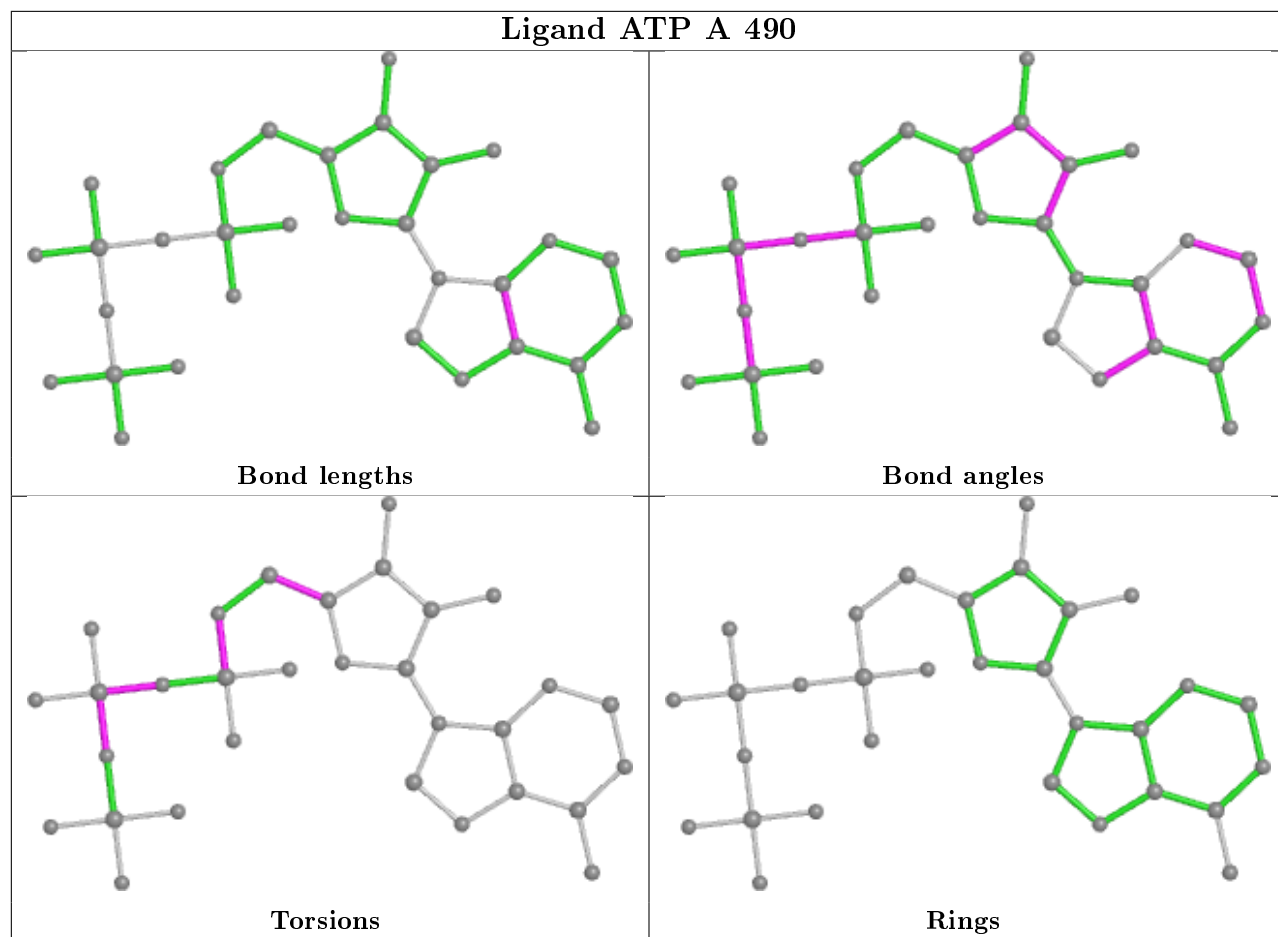
4 monomers are involved in 8 short contacts:

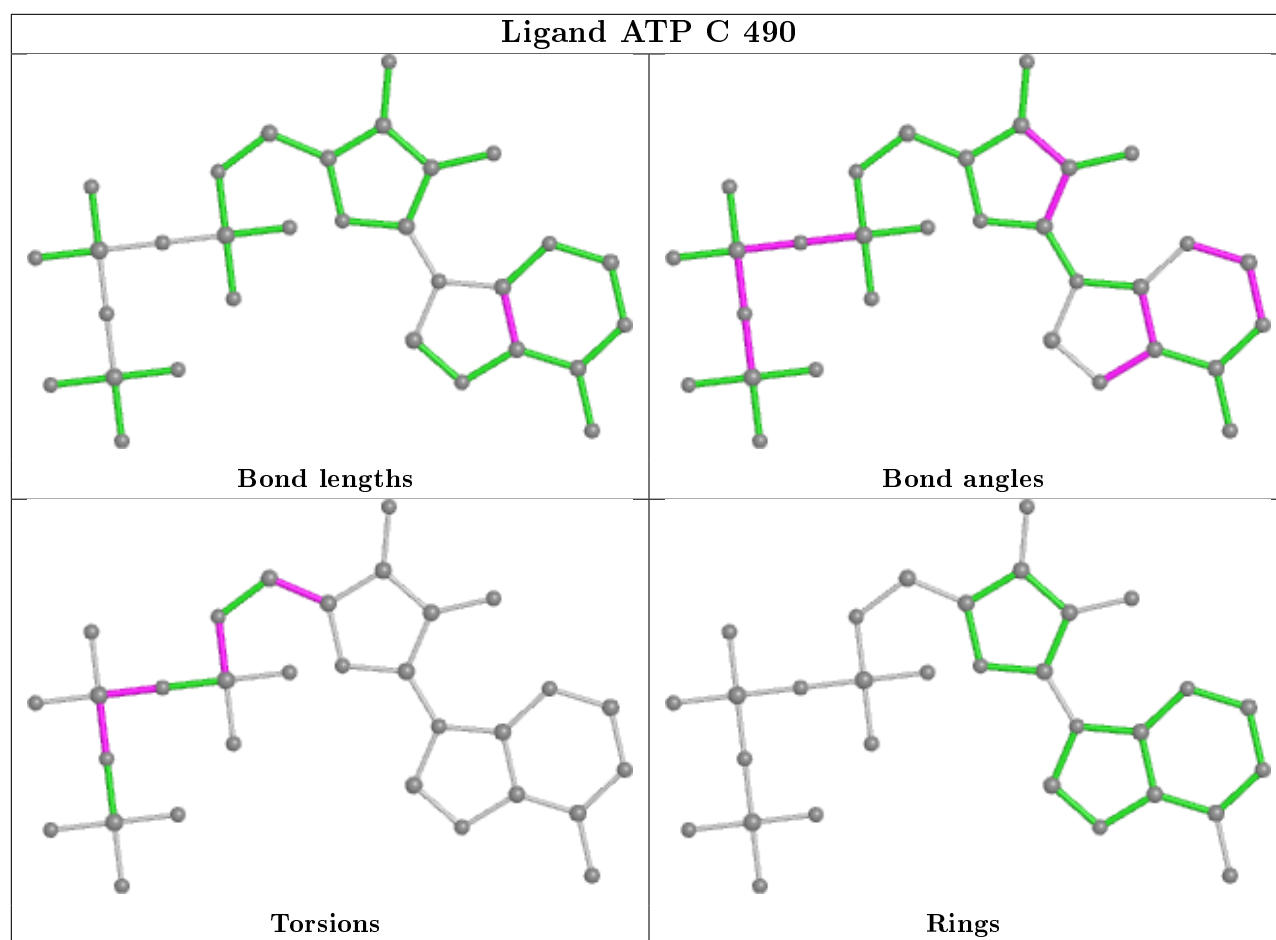
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	490	ATP	2	0
2	D	490	ATP	2	0
2	A	490	ATP	2	0
2	C	490	ATP	2	0

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 ⓘ

### 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	427/498 (85%)	-0.16	11 (2%) 56 54	33, 57, 114, 161	38 (8%)
1	B	430/498 (86%)	-0.16	6 (1%) 75 74	34, 56, 113, 165	32 (7%)
1	C	430/498 (86%)	-0.20	5 (1%) 79 77	33, 56, 115, 165	37 (8%)
1	D	430/498 (86%)	-0.15	5 (1%) 79 77	33, 56, 115, 177	31 (7%)
All	All	1717/1992 (86%)	-0.17	27 (1%) 72 70	33, 56, 116, 177	138 (8%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	327	PRO	7.0
1	A	264	SER	6.5
1	C	379	ASN	5.5
1	B	264	SER	4.6
1	C	264	SER	4.1
1	B	442	THR	3.6
1	D	378	GLU	3.6
1	A	49	ALA	3.4
1	A	221	PHE	3.3
1	D	380	ASN	3.3
1	A	481	GLU	3.3
1	A	263	SER	3.0
1	B	263	SER	2.8
1	A	483	LEU	2.6
1	A	10	GLY	2.6
1	B	10	GLY	2.6
1	B	9	TYR	2.5
1	D	221	PHE	2.5
1	A	482	ARG	2.5
1	A	308	ASN	2.4
1	A	486	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	308	ASN	2.3
1	B	477	GLU	2.3
1	C	258	THR	2.2
1	C	477	GLU	2.2
1	C	380	ASN	2.1
1	A	222	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

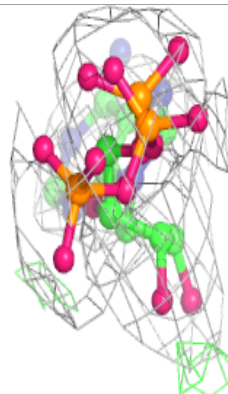
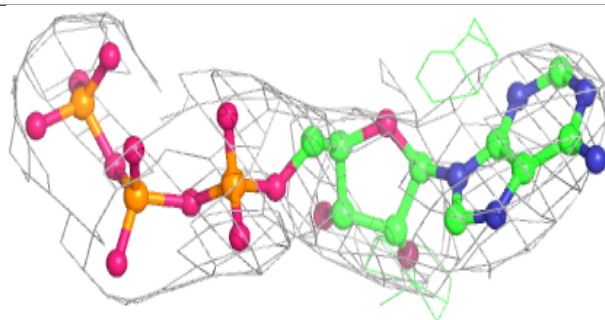
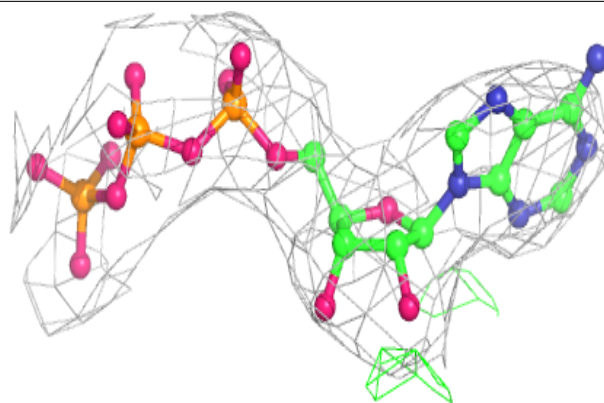
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	A	491	1/1	0.96	0.20	39,39,39,39	0
2	ATP	A	490	31/31	0.96	0.20	16,52,69,106	0
2	ATP	B	490	31/31	0.97	0.19	15,51,70,110	0
3	CA	B	491	1/1	0.97	0.19	42,42,42,42	0
2	ATP	D	490	31/31	0.97	0.19	15,52,73,107	0
3	CA	D	491	1/1	0.97	0.17	45,45,45,45	0
2	ATP	C	490	31/31	0.97	0.17	16,50,73,108	0
3	CA	C	491	1/1	0.98	0.15	45,45,45,45	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.

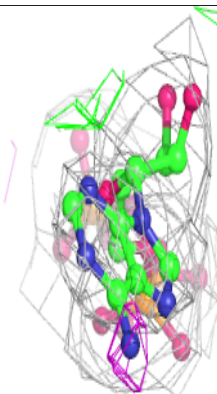
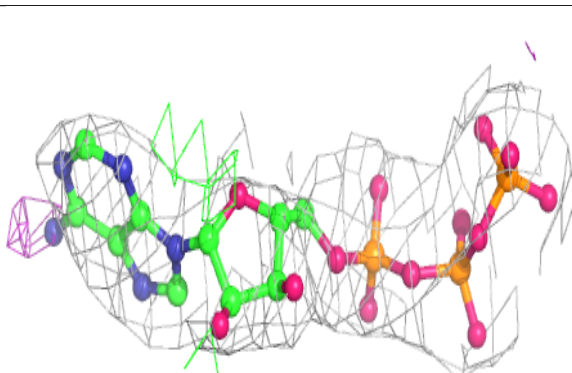
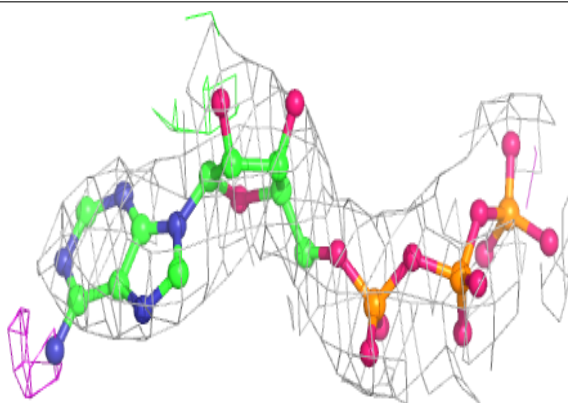


**Electron density around ATP A 490:**

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

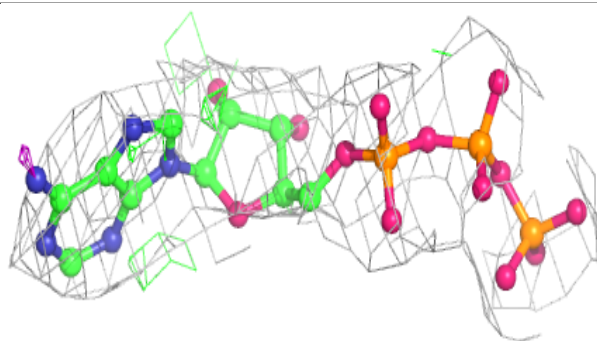
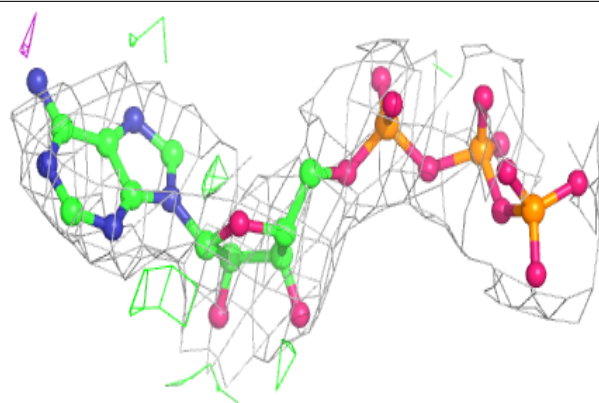
**Electron density around ATP B 490:**

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

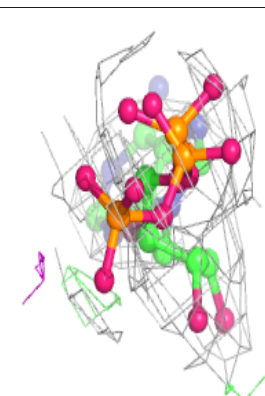
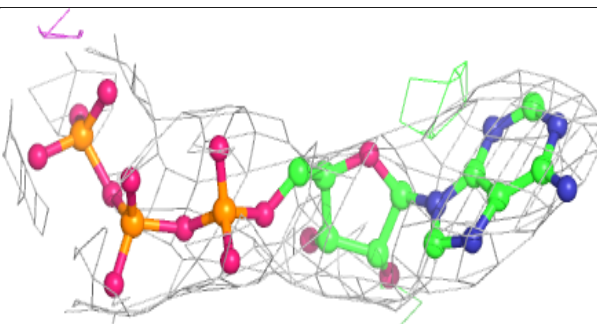
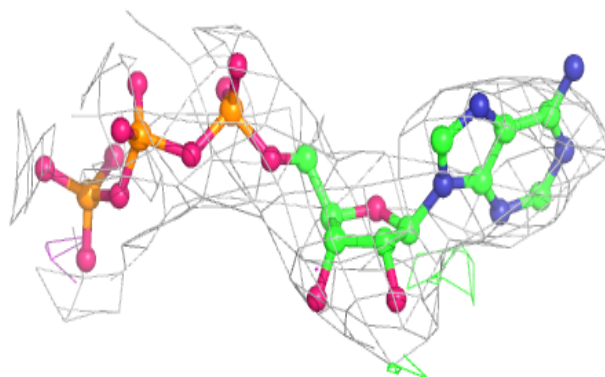


**Electron density around ATP D 490:**

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

**Electron density around ATP C 490:**

$2mF_o-DF_c$  (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.