



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:57 PM GMT

PDB ID : 1MV5  
Title : Crystal structure of LmrA ATP-binding domain  
Authors : Yuan, Y.; Chen, H.; Patel, D.  
Deposited on : 2002-09-24  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

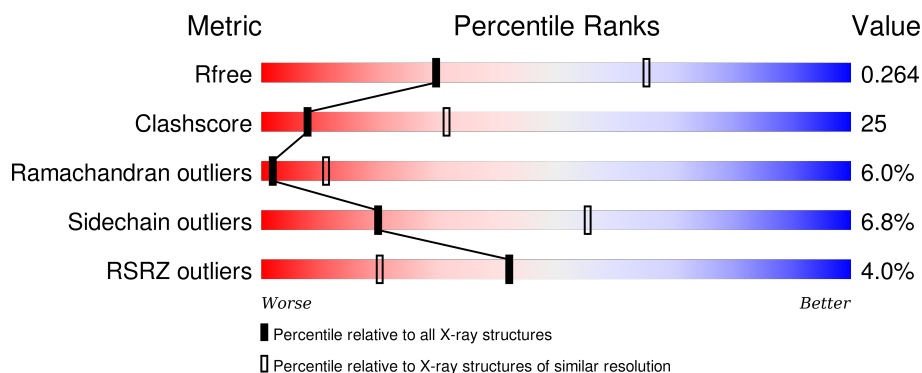
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	243	<div> <div>5%</div> <div>57% 35% 5%</div> </div>
1	B	243	<div> <div>3%</div> <div>59% 31% 9%</div> </div>
1	C	243	<div> <div>4%</div> <div>53% 38% 6%</div> </div>
1	D	243	<div> <div>4%</div> <div>49% 41% 8%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7671 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 Multidrug resistance ABC transporter ATP-binding and per-mease protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1866	1174	321	365	6			
1	B	242	Total	C	N	O	S	0	0	0
			1877	1179	320	372	6			
1	C	242	Total	C	N	O	S	0	0	0
			1862	1172	321	363	6			
1	D	241	Total	C	N	O	S	0	0	0
			1870	1175	320	369	6			

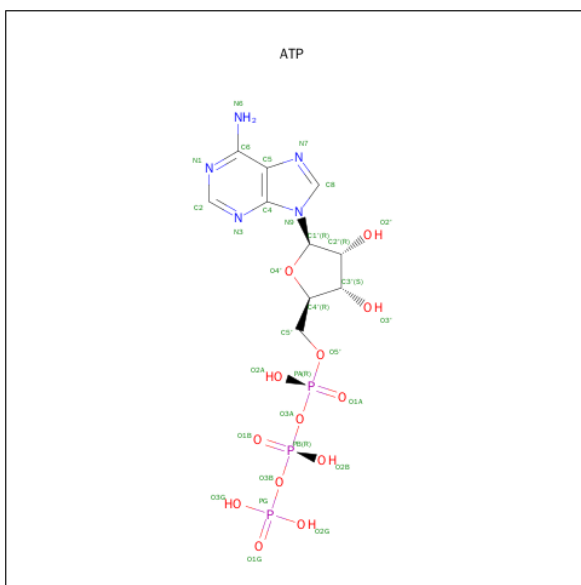
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	342	MET	-	INITIATING MET	UNP Q9CHL8
B	1342	MET	-	INITIATING MET	UNP Q9CHL8
C	2342	MET	-	INITIATING MET	UNP Q9CHL8
D	3342	MET	-	INITIATING MET	UNP Q9CHL8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

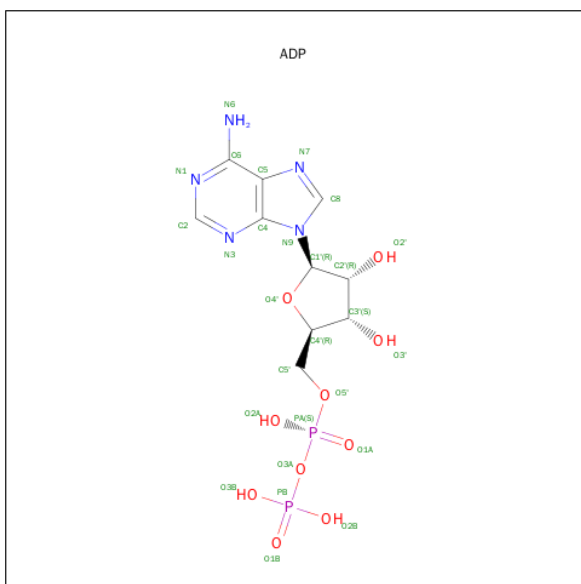
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 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>).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

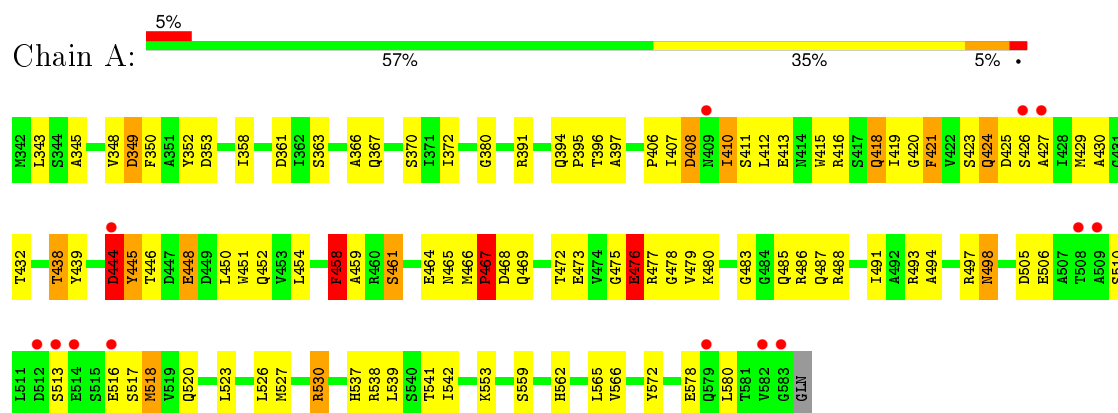
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	B	12	Total	O	0	0
			12	12		
5	C	24	Total	O	0	0
			24	24		
5	D	19	Total	O	0	0
			19	19		

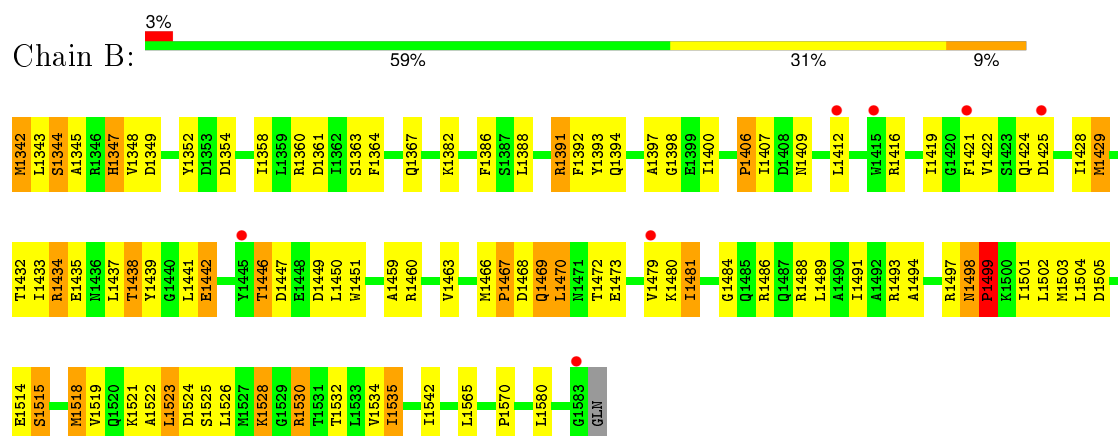
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

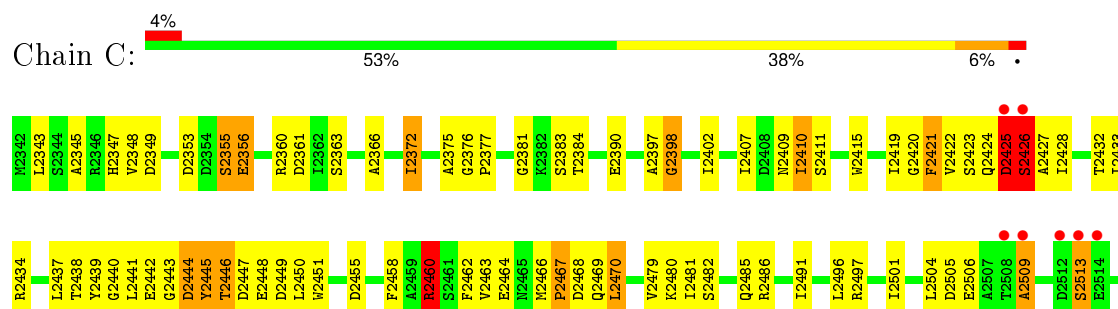
- Molecule 1: Multidrug resistance ABC transporter ATP-binding and permease protein



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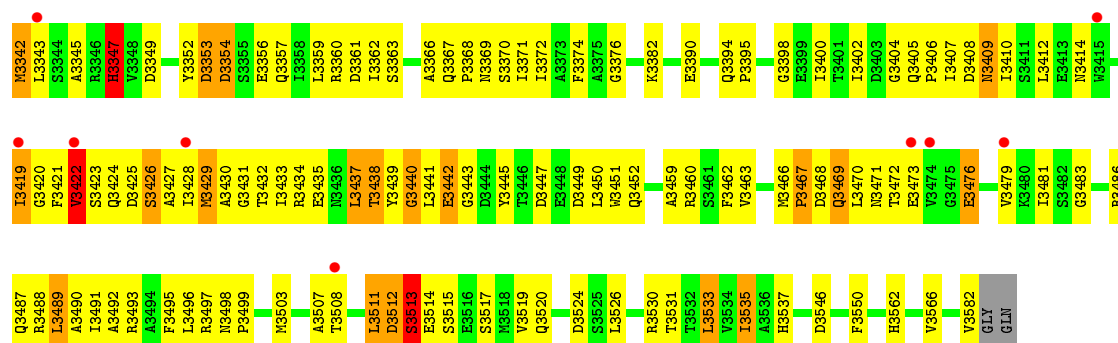


- Molecule 1: Multidrug resistance ABC transporter ATP-binding and permease protein





- Molecule 1: Multidrug resistance ABC transporter ATP-binding and permease protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.87Å 141.87Å 120.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.10 28.73 – 3.11	Depositor EDS
% Data completeness (in resolution range)	84.8 (40.00-3.10) 95.5 (28.73-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 3.11Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.251 , 0.283 0.242 , 0.264	Depositor DCC
$R_{free}$ test set	1192 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 16.2	EDS
Estimated twinning fraction	0.478 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 23832 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ATP, ADP

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	0.99	2/1897 (0.1%)	1.11	6/2566 (0.2%)
1	B	0.98	1/1908 (0.1%)	1.18	11/2580 (0.4%)
1	C	0.93	2/1893 (0.1%)	1.12	10/2561 (0.4%)
1	D	1.00	2/1901 (0.1%)	1.14	8/2570 (0.3%)
All	All	0.97	7/7599 (0.1%)	1.14	35/10277 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	ASP	CB-CG	8.63	1.69	1.51
1	B	1342	MET	SD-CE	6.14	2.12	1.77
1	C	2506	GLU	CG-CD	6.08	1.61	1.51
1	C	2445	TYR	CB-CG	5.82	1.60	1.51
1	A	518	MET	SD-CE	5.67	2.09	1.77
1	D	3342	MET	SD-CE	-5.55	1.46	1.77
1	D	3429	MET	CG-SD	5.09	1.94	1.81

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3450	LEU	CB-CG-CD1	-8.51	96.54	111.00
1	C	2533	LEU	CA-CB-CG	8.09	133.90	115.30
1	B	1470	LEU	CA-CB-CG	7.94	133.57	115.30
1	C	2426	SER	N-CA-C	-7.69	90.22	111.00
1	C	2445	TYR	CB-CA-C	7.50	125.39	110.40
1	B	1467	PRO	N-CA-C	7.37	131.26	112.10
1	B	1505	ASP	N-CA-C	-7.17	91.65	111.00
1	B	1518	MET	CB-CG-SD	-6.96	91.51	112.40
1	D	3512	ASP	N-CA-C	-6.71	92.88	111.00
1	A	438	THR	N-CA-C	6.68	129.03	111.00
1	B	1535	ILE	N-CA-C	-6.59	93.21	111.00
1	D	3533	LEU	CA-CB-CG	6.50	130.24	115.30
1	C	2425	ASP	N-CA-C	6.42	128.34	111.00
1	C	2425	ASP	CA-C-N	-6.28	103.39	117.20
1	B	1468	ASP	N-CA-C	-6.04	94.70	111.00
1	C	2509	ALA	N-CA-C	5.89	126.92	111.00
1	B	1470	LEU	CB-CG-CD2	-5.80	101.14	111.00
1	A	539	LEU	CA-CB-CG	5.79	128.61	115.30
1	D	3420	GLY	N-CA-C	-5.73	98.77	113.10
1	D	3419	ILE	CG1-CB-CG2	-5.68	98.91	111.40
1	D	3352	TYR	CA-CB-CG	5.66	124.14	113.40
1	D	3422	VAL	CA-C-N	-5.62	104.83	117.20
1	C	2534	VAL	CB-CA-C	-5.61	100.75	111.40
1	A	444	ASP	CB-CG-OD1	5.60	123.34	118.30
1	D	3535	ILE	N-CA-C	-5.54	96.05	111.00
1	C	2470	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	410	ILE	CB-CA-C	5.46	122.53	111.60
1	C	2425	ASP	C-N-CA	5.43	135.27	121.70
1	B	1528	LYS	N-CA-C	5.16	124.94	111.00
1	B	1565	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	1499	PRO	N-CA-C	5.15	125.49	112.10
1	A	445	TYR	CB-CA-C	5.15	120.70	110.40
1	B	1523	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	A	478	GLY	N-CA-C	-5.11	100.33	113.10
1	C	2535	ILE	N-CA-C	-5.04	97.38	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	2572	TYR	Sidechain
1	D	3422	VAL	Mainchain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	1866	0	1823	77	0
1	B	1877	0	1846	74	0
1	C	1862	0	1819	103	0
1	D	1870	0	1840	132	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	2	0
3	C	31	0	12	3	0
4	B	27	0	12	2	0
4	D	27	0	12	1	0
5	A	23	0	0	1	0
5	B	12	0	0	1	0
5	C	24	0	0	5	0
5	D	19	0	0	1	0
All	All	7671	0	7376	374	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 25.

All (374) 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:D:3466:MET:CE	1:D:3466:MET:SD	2.04	1.45
1:A:429:MET:SD	1:A:429:MET:CE	2.05	1.43
1:A:518:MET:SD	1:A:518:MET:CE	2.09	1.40
1:B:1342:MET:SD	1:B:1342:MET:CE	2.12	1.38
1:C:2539:LEU:HD11	5:C:4069:HOH:O	1.34	1.21
1:C:2438:THR:O	1:C:2441:LEU:HG	1.45	1.16
1:D:3342:MET:HE3	1:D:3367:GLN:HG2	1.21	1.14
1:D:3353:ASP:O	1:D:3354:ASP:CB	1.98	1.09
1:C:2518:MET:HA	1:C:2521:LYS:HE2	1.35	1.08
1:D:3353:ASP:O	1:D:3354:ASP:HB3	1.51	1.07
1:C:2446:THR:O	1:C:2449:ASP:OD1	1.69	1.07
1:D:3441:LEU:O	1:D:3497:ARG:NH2	1.95	0.99
1:D:3422:VAL:HG21	1:D:3490:ALA:HB1	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1491:ILE:HG21	1:B:1522:ALA:HB1	1.46	0.96
1:D:3342:MET:HE3	1:D:3367:GLN:CG	1.97	0.94
1:C:2440:GLY:O	1:C:2441:LEU:HD23	1.68	0.93
1:C:2518:MET:CA	1:C:2521:LYS:HE2	2.00	0.92
1:A:439:TYR:H	1:A:493:ARG:HH12	1.17	0.90
1:D:3370:SER:HB2	1:D:3546:ASP:OD2	1.70	0.90
1:A:427:ALA:HB3	1:A:486:ARG:NH1	1.89	0.88
4:B:1600:ADP:H2'	1:C:2353:ASP:OD2	1.75	0.86
1:C:2563:ASN:OD1	1:C:2564:GLU:N	2.08	0.86
1:D:3441:LEU:CD1	1:D:3496:LEU:HD12	2.08	0.83
1:D:3342:MET:CE	1:D:3367:GLN:HG2	2.08	0.82
1:A:427:ALA:HB3	1:A:486:ARG:CZ	2.10	0.82
1:D:3422:VAL:CG2	1:D:3490:ALA:HB1	2.10	0.81
1:C:2518:MET:HA	1:C:2521:LYS:CE	2.11	0.80
1:D:3515:SER:O	1:D:3519:VAL:CG2	2.28	0.80
1:D:3515:SER:O	1:D:3519:VAL:HG23	1.80	0.80
1:C:2460:ARG:NH2	1:D:3428:ILE:HA	1.97	0.80
1:B:1481:ILE:HB	1:B:1486:ARG:HE	1.45	0.80
1:D:3343:LEU:HB3	1:D:3366:ALA:HB3	1.63	0.79
1:A:438:THR:O	1:A:438:THR:HG22	1.82	0.79
1:D:3441:LEU:CD1	1:D:3496:LEU:CD1	2.61	0.79
1:C:2349:ASP:HB2	1:C:2397:ALA:HB3	1.65	0.78
1:B:1526:LEU:HD22	1:B:1530:ARG:HH22	1.47	0.77
1:C:2518:MET:CB	1:C:2521:LYS:HE2	2.14	0.77
1:D:3431:GLY:O	1:D:3473:GLU:HG2	1.85	0.77
1:D:3422:VAL:HG11	1:D:3490:ALA:CB	2.14	0.77
1:B:1344:SER:OG	5:B:4063:HOH:O	1.97	0.77
1:D:3353:ASP:O	1:D:3354:ASP:HB2	1.85	0.76
1:B:1434:ARG:HB2	1:B:1470:LEU:O	1.86	0.75
1:C:2449:ASP:OD1	1:C:2450:LEU:N	2.19	0.75
1:A:424:GLN:CG	1:A:486:ARG:HH21	1.99	0.75
1:C:2460:ARG:HH21	1:D:3428:ILE:HA	1.50	0.75
1:B:1519:VAL:O	1:B:1523:LEU:HB2	1.87	0.74
1:A:506:GLU:HG3	1:A:537:HIS:HB2	1.68	0.74
1:C:2455:ASP:O	1:D:3439:TYR:OH	2.06	0.73
1:C:2360:ARG:NH2	1:C:2553:LYS:O	2.22	0.73
1:A:424:GLN:HG2	1:A:486:ARG:HH21	1.54	0.73
1:D:3515:SER:O	1:D:3519:VAL:CB	2.36	0.73
1:D:3441:LEU:HD11	1:D:3496:LEU:HD12	1.71	0.72
1:D:3515:SER:O	1:D:3519:VAL:HB	1.88	0.72
1:B:1421:PHE:CD1	1:B:1499:PRO:HG2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3442:GLU:H	1:D:3445:TYR:HE1	1.36	0.71
1:C:2518:MET:HA	1:C:2521:LYS:HG2	1.73	0.71
1:D:3491:ILE:HG23	1:D:3526:LEU:HD22	1.71	0.71
1:B:1400:ILE:HB	1:B:1407:ILE:HD12	1.72	0.71
1:A:526:LEU:O	1:A:530:ARG:HD3	1.90	0.70
1:B:1484:GLY:HA2	1:B:1518:MET:SD	2.32	0.69
1:D:3442:GLU:HB2	1:D:3445:TYR:OH	1.92	0.69
1:B:1491:ILE:O	1:B:1494:ALA:HB3	1.93	0.69
1:D:3422:VAL:CB	1:D:3490:ALA:HB1	2.24	0.67
1:B:1386:PHE:HE1	1:B:1504:LEU:O	1.77	0.67
1:B:1437:LEU:HD13	1:B:1489:LEU:HD22	1.76	0.67
1:C:2557:THR:HG22	5:C:4034:HOH:O	1.94	0.67
1:A:488:ARG:NH2	1:A:518:MET:HB2	2.10	0.67
1:D:3429:MET:O	1:D:3429:MET:HG3	1.94	0.66
1:C:2518:MET:HG2	1:C:2521:LYS:NZ	2.11	0.66
1:D:3421:PHE:HZ	1:D:3424:GLN:NE2	1.94	0.65
1:A:465:ASN:ND2	1:B:1422:VAL:HB	2.11	0.65
1:C:2415:TRP:CE2	1:C:2419:ILE:HD11	2.32	0.65
1:D:3462:PHE:CZ	1:D:3488:ARG:NH1	2.64	0.65
1:D:3437:LEU:HD21	1:D:3489:LEU:HD23	1.78	0.65
1:B:1466:MET:HB3	1:B:1472:THR:HG21	1.79	0.64
1:C:2424:GLN:HG3	1:C:2425:ASP:H	1.62	0.64
1:A:479:VAL:HG12	1:A:480:LYS:H	1.62	0.64
1:A:446:THR:HG22	1:A:448:GLU:H	1.61	0.64
1:D:3511:LEU:O	1:D:3513:SER:N	2.31	0.64
1:B:1347:HIS:O	1:B:1398:GLY:HA3	1.97	0.64
1:D:3462:PHE:HZ	1:D:3488:ARG:HH12	1.46	0.63
1:C:2557:THR:CG2	5:C:4034:HOH:O	2.46	0.63
1:B:1493:ARG:HH21	1:B:1497:ARG:NH2	1.97	0.63
1:D:3441:LEU:HD13	1:D:3496:LEU:HD13	1.80	0.62
1:D:3422:VAL:HG11	1:D:3490:ALA:HB2	1.81	0.62
1:C:2463:VAL:HA	1:C:2466:MET:HE2	1.81	0.62
1:D:3342:MET:HG3	1:D:3366:ALA:O	1.99	0.62
1:A:391:ARG:NH2	1:A:411:SER:O	2.33	0.62
1:A:348:VAL:HG13	1:A:395:PRO:HB3	1.81	0.62
1:C:2518:MET:HG2	1:C:2521:LYS:HE2	1.81	0.62
1:A:479:VAL:HG12	1:A:480:LYS:N	2.15	0.62
1:C:2438:THR:O	1:C:2441:LEU:CG	2.36	0.61
1:D:3441:LEU:C	1:D:3497:ARG:HH21	2.02	0.61
1:D:3433:ILE:HD12	1:D:3469:GLN:O	1.99	0.61
1:A:432:THR:HA	1:A:472:THR:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:PRO:HD3	1:B:1392:PHE:CE1	2.35	0.61
1:D:3562:HIS:O	1:D:3566:VAL:HG23	2.00	0.61
1:D:3342:MET:CG	1:D:3366:ALA:O	2.49	0.61
1:D:3432:THR:HG23	1:D:3471:ASN:HA	1.83	0.61
1:D:3422:VAL:HG13	1:D:3425:ASP:HB2	1.83	0.61
1:C:2513:SER:CB	1:C:2540:SER:H	2.14	0.60
1:D:3499:PRO:HD2	1:D:3530:ARG:NH1	2.17	0.60
1:A:406:PRO:O	1:A:410:ILE:HB	2.02	0.60
1:B:1484:GLY:O	1:B:1488:ARG:HG3	2.02	0.60
1:D:3410:ILE:HG22	1:D:3412:LEU:H	1.67	0.60
1:B:1345:ALA:HB3	1:B:1364:PHE:H	1.67	0.60
1:B:1391:ARG:O	1:B:1391:ARG:HG3	2.01	0.59
1:D:3582:VAL:HB	5:D:4054:HOH:O	2.00	0.59
1:A:439:TYR:H	1:A:493:ARG:NH1	1.95	0.59
1:C:2419:ILE:HG22	1:C:2420:GLY:N	2.17	0.59
1:C:2348:VAL:HA	1:C:2398:GLY:HA3	1.85	0.59
1:B:1433:ILE:HD12	1:B:1472:THR:HB	1.85	0.59
1:A:427:ALA:H	1:A:486:ARG:HH12	1.49	0.59
1:C:2518:MET:CG	1:C:2521:LYS:HE2	2.33	0.59
1:A:438:THR:CG2	1:A:438:THR:O	2.51	0.59
1:B:1421:PHE:HE1	1:B:1497:ARG:HD2	1.68	0.58
1:B:1434:ARG:NH2	1:B:1447:ASP:OD1	2.36	0.58
1:A:424:GLN:NE2	1:A:487:GLN:HA	2.19	0.58
1:D:3430:ALA:HB1	1:D:3435:GLU:HB3	1.84	0.58
1:C:2455:ASP:HA	1:D:3439:TYR:OH	2.04	0.58
1:B:1433:ILE:CD1	1:B:1472:THR:HB	2.33	0.58
1:C:2520:GLN:HG3	1:C:2538:ARG:NH1	2.18	0.58
1:D:3441:LEU:CD1	1:D:3496:LEU:HD13	2.32	0.58
1:D:3511:LEU:C	1:D:3513:SER:N	2.57	0.58
1:A:491:ILE:HG23	1:A:526:LEU:HD22	1.86	0.58
1:C:2518:MET:HG2	1:C:2521:LYS:CE	2.34	0.57
1:D:3433:ILE:HD13	1:D:3463:VAL:HG13	1.86	0.57
1:C:2479:VAL:HG12	1:C:2480:LYS:N	2.18	0.57
1:C:2447:ASP:HB2	1:C:2470:LEU:CD1	2.34	0.57
1:D:3441:LEU:HB3	1:D:3445:TYR:CE1	2.39	0.57
1:D:3366:ALA:HA	1:D:3372:ILE:HD13	1.86	0.57
1:B:1526:LEU:HD22	1:B:1530:ARG:NH2	2.19	0.57
1:D:3357:GLN:CD	1:D:3360:ARG:HG2	2.25	0.57
1:A:444:ASP:HB2	1:A:450:LEU:HD21	1.87	0.57
1:D:3422:VAL:CG1	1:D:3490:ALA:CB	2.82	0.57
1:D:3437:LEU:HA	1:D:3493:ARG:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ASP:OD1	4:D:3600:ADP:H2'	2.04	0.57
1:C:2437:LEU:O	1:C:2496:LEU:HD23	2.05	0.56
1:A:498:ASN:HD22	1:A:530:ARG:NH2	2.02	0.56
1:B:1342:MET:SD	1:B:1367:GLN:HG2	2.46	0.56
3:A:601:ATP:O2'	1:D:3356:GLU:OE1	2.22	0.56
1:C:2518:MET:HG2	1:C:2521:LYS:HZ1	1.70	0.55
1:C:2538:ARG:HB2	1:C:2541:THR:OG1	2.06	0.55
1:A:416:ARG:O	1:A:497:ARG:NH2	2.39	0.55
1:A:473:GLU:O	1:A:479:VAL:HG23	2.07	0.55
1:B:1493:ARG:HH21	1:B:1497:ARG:HH21	1.53	0.55
1:D:3433:ILE:O	1:D:3437:LEU:HG	2.07	0.55
1:D:3405:GLN:NE2	1:D:3409:ASN:ND2	2.54	0.55
1:C:2445:TYR:O	1:C:2449:ASP:HB3	2.07	0.55
1:C:2479:VAL:HG12	1:C:2480:LYS:H	1.72	0.55
1:C:2440:GLY:C	1:C:2441:LEU:HD23	2.26	0.55
1:B:1514:GLU:O	1:B:1518:MET:HG3	2.07	0.55
1:C:2415:TRP:NE1	1:C:2419:ILE:HD11	2.22	0.55
1:D:3359:LEU:HD22	1:D:3362:ILE:HD12	1.88	0.55
1:C:2518:MET:HA	1:C:2521:LYS:CG	2.36	0.54
1:D:3371:ILE:HG22	1:D:3372:ILE:N	2.21	0.54
1:A:372:ILE:O	1:A:372:ILE:HG13	2.07	0.54
1:C:2381:GLY:HA2	3:C:2601:ATP:O2A	2.07	0.54
1:A:407:ILE:HG13	1:A:408:ASP:N	2.22	0.54
1:A:464:GLU:C	1:A:466:MET:H	2.09	0.54
1:B:1421:PHE:O	1:B:1503:MET:HB2	2.08	0.53
1:C:2446:THR:CG2	1:C:2447:ASP:N	2.71	0.53
1:C:2428:ILE:HG12	1:C:2486:ARG:HH12	1.73	0.53
1:B:1469:GLN:O	1:B:1470:LEU:HB3	2.08	0.53
1:A:523:LEU:O	1:A:527:MET:HG3	2.08	0.53
1:D:3438:THR:O	1:D:3438:THR:CG2	2.56	0.53
1:D:3419:ILE:CG1	1:D:3499:PRO:HG2	2.38	0.53
1:D:3459:ALA:HA	1:D:3462:PHE:CE1	2.43	0.53
1:B:1498:ASN:N	1:B:1499:PRO:HD3	2.24	0.53
1:D:3514:GLU:C	1:D:3517:SER:H	2.12	0.53
1:B:1459:ALA:O	1:B:1463:VAL:HG23	2.09	0.53
1:A:391:ARG:NH2	1:A:407:ILE:O	2.39	0.53
1:B:1419:ILE:CG2	1:B:1501:ILE:HD12	2.38	0.53
1:D:3481:ILE:HG22	1:D:3483:GLY:H	1.74	0.53
1:C:2424:GLN:CG	1:C:2425:ASP:H	2.21	0.53
1:C:2518:MET:HA	1:C:2521:LYS:CD	2.40	0.52
1:B:1429:MET:SD	1:B:1493:ARG:NH1	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1432:THR:HB	1:B:1435:GLU:HB2	1.92	0.52
1:A:415:TRP:NE1	1:A:419:ILE:HD11	2.24	0.52
1:C:2355:SER:O	1:C:2356:GLU:HB2	2.10	0.52
1:C:2372:ILE:HG12	1:C:2533:LEU:HB3	1.92	0.52
1:D:3442:GLU:HB2	1:D:3445:TYR:CZ	2.45	0.52
1:B:1421:PHE:CD2	1:B:1502:LEU:HD12	2.45	0.51
1:B:1447:ASP:CG	1:B:1470:LEU:HD21	2.30	0.51
1:B:1345:ALA:O	1:B:1363:SER:HA	2.10	0.51
1:A:419:ILE:HG22	1:A:420:GLY:N	2.26	0.51
1:A:423:SER:OG	1:A:505:ASP:HB3	2.11	0.51
1:A:427:ALA:CB	1:A:486:ARG:NH1	2.68	0.51
1:A:491:ILE:O	1:A:494:ALA:HB3	2.11	0.51
1:D:3422:VAL:HG22	1:D:3425:ASP:OD2	2.10	0.51
1:D:3512:ASP:O	1:D:3515:SER:N	2.41	0.51
1:D:3428:ILE:HD12	1:D:3493:ARG:HH12	1.76	0.51
1:D:3405:GLN:NE2	1:D:3409:ASN:HD21	2.09	0.51
1:A:439:TYR:HB2	1:A:493:ARG:HH22	1.75	0.51
1:B:1424:GLN:HE22	1:B:1493:ARG:CZ	2.25	0.50
1:D:3419:ILE:HG12	1:D:3499:PRO:HG2	1.94	0.50
1:C:2428:ILE:HG12	1:C:2486:ARG:NH1	2.27	0.50
1:D:3422:VAL:HG11	1:D:3490:ALA:HB1	1.92	0.50
1:B:1349:ASP:HB2	1:B:1397:ALA:HB3	1.93	0.50
1:D:3347:HIS:H	1:D:3363:SER:HB3	1.75	0.50
1:C:2443:GLY:O	1:C:2444:ASP:HB2	2.12	0.50
1:D:3422:VAL:CB	1:D:3490:ALA:CB	2.89	0.50
1:A:479:VAL:HG13	1:B:1392:PHE:HB3	1.92	0.50
1:C:2345:ALA:O	1:C:2363:SER:HA	2.11	0.50
1:B:1521:LYS:O	1:B:1524:ASP:HB2	2.12	0.50
1:A:565:LEU:HB3	1:A:572:TYR:CD2	2.46	0.50
1:B:1473:GLU:O	1:B:1479:VAL:HB	2.12	0.50
1:D:3407:ILE:C	1:D:3409:ASN:H	2.15	0.50
1:D:3514:GLU:O	1:D:3517:SER:N	2.44	0.49
1:B:1348:VAL:O	1:B:1360:ARG:O	2.29	0.49
1:D:3427:ALA:HB2	1:D:3486:ARG:NH1	2.27	0.49
1:D:3345:ALA:O	1:D:3363:SER:HA	2.13	0.49
1:B:1441:LEU:O	1:B:1442:GLU:HB2	2.12	0.49
1:D:3439:TYR:O	1:D:3441:LEU:HG	2.12	0.49
1:C:2447:ASP:HB2	1:C:2470:LEU:HD12	1.95	0.49
1:D:3439:TYR:O	1:D:3440:GLY:C	2.51	0.49
1:D:3421:PHE:CZ	1:D:3424:GLN:NE2	2.78	0.49
1:C:2562:HIS:O	1:C:2566:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2542:ILE:HG23	1:C:2548:ILE:HG12	1.94	0.49
1:C:2446:THR:CG2	1:C:2447:ASP:H	2.25	0.48
1:C:2432:THR:HG22	1:C:2433:ILE:N	2.28	0.48
1:B:1493:ARG:NH2	1:B:1497:ARG:NH2	2.61	0.48
1:A:448:GLU:OE2	1:A:452:GLN:NE2	2.46	0.48
1:D:3432:THR:HG22	1:D:3434:ARG:HB3	1.96	0.48
1:A:444:ASP:O	1:A:445:TYR:CD2	2.66	0.48
1:A:517:SER:O	1:A:520:GLN:HB2	2.13	0.48
1:C:2481:ILE:HG22	1:C:2482:SER:O	2.13	0.48
1:C:2446:THR:HG22	1:C:2447:ASP:N	2.29	0.48
1:D:3431:GLY:C	1:D:3473:GLU:HA	2.34	0.48
1:B:1515:SER:O	1:B:1519:VAL:HB	2.14	0.48
1:C:2505:ASP:HB3	1:C:2535:ILE:HB	1.95	0.48
1:C:2526:LEU:O	1:C:2530:ARG:HD2	2.14	0.48
1:A:517:SER:CB	5:A:4065:HOH:O	2.61	0.48
1:A:421:PHE:CD2	1:A:421:PHE:C	2.87	0.48
1:C:2520:GLN:HG3	1:C:2538:ARG:HH12	1.78	0.47
1:D:3347:HIS:O	1:D:3398:GLY:HA3	2.14	0.47
1:A:352:TYR:HD2	1:A:358:ILE:HG13	1.78	0.47
1:B:1386:PHE:CE1	1:B:1504:LEU:O	2.63	0.47
1:C:2419:ILE:HG22	1:C:2420:GLY:H	1.80	0.47
1:C:2384:THR:OG1	3:C:2601:ATP:O2A	2.26	0.47
1:B:1446:THR:HB	1:B:1449:ASP:HB2	1.96	0.47
1:A:485:GLN:NE2	1:B:1416:ARG:HH11	2.11	0.47
1:C:2455:ASP:CA	1:D:3439:TYR:OH	2.63	0.47
1:A:350:PHE:HA	1:A:396:THR:HG23	1.96	0.47
1:D:3370:SER:CB	1:D:3546:ASP:OD2	2.55	0.47
1:C:2424:GLN:CG	1:C:2425:ASP:N	2.78	0.47
1:C:2479:VAL:CG1	1:C:2480:LYS:H	2.27	0.47
1:B:1441:LEU:O	1:B:1442:GLU:CB	2.63	0.47
1:A:542:ILE:HD12	1:A:580:LEU:HD21	1.96	0.47
1:C:2421:PHE:HD2	1:C:2422:VAL:N	2.13	0.47
1:B:1481:ILE:HG13	1:B:1486:ARG:HH21	1.80	0.47
1:A:394:GLN:OE1	1:A:408:ASP:OD2	2.33	0.46
1:C:2347:HIS:ND1	1:C:2361:ASP:OD2	2.48	0.46
1:D:3407:ILE:HG22	1:D:3407:ILE:O	2.14	0.46
1:C:2421:PHE:CD2	1:C:2421:PHE:C	2.89	0.46
1:C:2377:PRO:HG3	1:C:2579:GLN:HE22	1.80	0.46
1:C:2518:MET:CA	1:C:2521:LYS:HG2	2.44	0.46
1:A:475:GLY:O	1:A:477:ARG:N	2.48	0.46
1:D:3492:ALA:O	1:D:3495:PHE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3366:ALA:HA	1:D:3372:ILE:CD1	2.46	0.46
1:D:3449:ASP:O	1:D:3452:GLN:HB2	2.15	0.46
1:D:3371:ILE:CG2	1:D:3372:ILE:N	2.79	0.46
1:B:1432:THR:HG22	1:B:1434:ARG:H	1.80	0.46
1:A:467:PRO:C	1:A:469:GLN:H	2.20	0.46
1:C:2497:ARG:NH1	5:C:4049:HOH:O	2.48	0.46
1:C:2451:TRP:CH2	1:C:2464:GLU:HG3	2.50	0.46
1:B:1502:LEU:HD23	1:B:1532:THR:HG23	1.98	0.45
1:A:380:GLY:N	3:A:601:ATP:O1B	2.50	0.45
1:A:345:ALA:O	1:A:363:SER:HA	2.17	0.45
1:D:3498:ASN:N	1:D:3499:PRO:HD3	2.32	0.45
1:D:3422:VAL:CG1	1:D:3490:ALA:HB1	2.46	0.45
1:C:2390:GLU:OE1	1:C:2421:PHE:HD1	2.00	0.45
1:A:418:GLN:HB3	1:A:418:GLN:HE21	1.57	0.45
1:D:3447:ASP:OD2	1:D:3470:LEU:HD12	2.17	0.45
1:A:424:GLN:HE22	1:A:487:GLN:HA	1.82	0.45
1:D:3514:GLU:HA	1:D:3517:SER:OG	2.17	0.45
1:C:2491:ILE:HG23	1:C:2526:LEU:HD22	1.98	0.45
1:A:421:PHE:C	1:A:421:PHE:HD2	2.21	0.45
1:A:349:ASP:HB2	1:A:397:ALA:HB3	1.98	0.45
1:B:1447:ASP:O	1:B:1451:TRP:CD1	2.70	0.44
1:B:1502:LEU:HD13	1:B:1530:ARG:NH2	2.33	0.44
1:D:3400:ILE:O	1:D:3407:ILE:HG13	2.17	0.44
1:A:458:PHE:N	1:A:458:PHE:HD2	2.15	0.44
1:D:3441:LEU:HA	1:D:3441:LEU:HD23	1.53	0.44
1:B:1429:MET:HE1	1:B:1493:ARG:NH1	2.32	0.44
1:C:2580:LEU:HD23	1:C:2580:LEU:HA	1.83	0.44
1:A:367:GLN:O	1:A:370:SER:OG	2.24	0.44
1:B:1352:TYR:CD1	1:B:1358:ILE:HD12	2.52	0.44
1:C:2421:PHE:CE2	1:C:2423:SER:HB3	2.52	0.44
1:A:458:PHE:CD2	1:A:458:PHE:N	2.86	0.44
1:C:2366:ALA:HB2	1:C:2372:ILE:HD13	1.99	0.44
1:C:2509:ALA:HA	5:C:4070:HOH:O	2.17	0.44
1:C:2479:VAL:CG1	1:C:2480:LYS:N	2.80	0.44
1:B:1446:THR:O	1:B:1450:LEU:HG	2.17	0.44
1:B:1343:LEU:HD12	1:B:1501:ILE:HD13	1.99	0.44
1:C:2410:ILE:HG13	1:C:2410:ILE:H	1.59	0.44
1:D:3376:GLY:HA2	1:D:3550:PHE:HE1	1.82	0.44
1:B:1434:ARG:HH11	1:B:1434:ARG:CG	2.30	0.44
1:B:1434:ARG:O	1:B:1438:THR:HB	2.18	0.44
1:D:3513:SER:O	1:D:3517:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2432:THR:HG22	1:C:2434:ARG:H	1.83	0.44
1:C:2407:ILE:HA	1:C:2410:ILE:HD12	1.99	0.43
1:C:2455:ASP:OD1	1:D:3439:TYR:OH	2.35	0.43
1:D:3374:PHE:O	1:D:3382:LYS:HG2	2.19	0.43
1:D:3488:ARG:C	1:D:3490:ALA:H	2.19	0.43
1:A:366:ALA:HB2	1:A:372:ILE:HD13	2.00	0.43
1:A:415:TRP:CE2	1:A:419:ILE:HD11	2.54	0.43
1:B:1424:GLN:HE22	1:B:1493:ARG:NE	2.17	0.43
1:B:1419:ILE:HG22	1:B:1501:ILE:HD12	2.01	0.43
1:B:1388:LEU:HD23	1:B:1393:TYR:HB2	2.01	0.43
1:D:3483:GLY:O	1:D:3487:GLN:HG3	2.19	0.43
1:D:3520:GLN:O	1:D:3524:ASP:CG	2.57	0.43
1:A:459:ALA:C	1:A:461:SER:H	2.21	0.43
1:A:366:ALA:HB2	1:A:372:ILE:CD1	2.49	0.43
1:B:1525:SER:HA	1:B:1528:LYS:HD2	2.00	0.43
1:A:480:LYS:NZ	1:B:1412:LEU:HD22	2.33	0.43
1:D:3402:ILE:C	1:D:3404:GLY:N	2.72	0.43
1:D:3451:TRP:HZ3	1:D:3460:ARG:O	2.01	0.43
1:B:1406:PRO:HB2	1:B:1409:ASN:ND2	2.34	0.42
1:D:3425:ASP:O	1:D:3426:SER:O	2.36	0.42
1:D:3390:GLU:HG2	1:D:3503:MET:HE1	2.02	0.42
1:D:3359:LEU:HD22	1:D:3362:ILE:CD1	2.49	0.42
1:D:3503:MET:HB2	1:D:3503:MET:HE2	1.90	0.42
1:A:488:ARG:HA	1:A:491:ILE:HD12	2.00	0.42
1:B:1542:ILE:HD12	1:B:1580:LEU:HD21	2.00	0.42
1:D:3489:LEU:O	1:D:3492:ALA:HB3	2.20	0.42
1:D:3409:ASN:C	1:D:3410:ILE:HG13	2.39	0.42
1:C:2577:SER:O	1:C:2581:THR:HB	2.19	0.42
1:C:2383:SER:HB2	3:C:2601:ATP:O1A	2.20	0.42
1:D:3476:GLU:HG3	1:D:3476:GLU:H	1.55	0.42
1:C:2449:ASP:OD1	1:C:2449:ASP:C	2.59	0.41
1:C:2376:GLY:HA3	1:C:2551:ILE:O	2.20	0.41
1:D:3357:GLN:NE2	1:D:3360:ARG:HG2	2.35	0.41
1:A:454:LEU:O	1:A:459:ALA:N	2.51	0.41
1:D:3488:ARG:HB2	1:D:3488:ARG:HE	1.59	0.41
1:D:3394:GLN:HA	1:D:3394:GLN:OE1	2.19	0.41
1:B:1433:ILE:HD11	1:B:1472:THR:HB	2.03	0.41
1:D:3432:THR:HA	1:D:3472:THR:O	2.21	0.41
1:D:3535:ILE:HG22	1:D:3537:HIS:CE1	2.56	0.41
1:A:479:VAL:CG1	1:A:480:LYS:H	2.30	0.41
1:D:3467:PRO:O	1:D:3468:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2402:ILE:HD12	1:C:2501:ILE:HD11	2.02	0.41
1:A:538:ARG:O	1:A:541:THR:HB	2.21	0.41
1:D:3407:ILE:HG21	1:D:3414:ASN:ND2	2.36	0.41
1:A:430:ALA:HB1	1:A:476:GLU:OE2	2.20	0.41
1:C:2409:ASN:HD22	1:C:2409:ASN:HA	1.62	0.41
1:B:1534:VAL:HG12	1:B:1535:ILE:N	2.35	0.41
1:C:2446:THR:HG23	1:C:2447:ASP:H	1.84	0.41
1:D:3421:PHE:CD2	1:D:3421:PHE:N	2.89	0.41
1:D:3514:GLU:O	1:D:3517:SER:OG	2.32	0.41
1:D:3468:ASP:HB3	1:D:3471:ASN:HB2	2.02	0.41
1:C:2481:ILE:HG23	1:C:2485:GLN:HB2	2.02	0.41
1:C:2409:ASN:O	1:C:2411:SER:N	2.53	0.41
1:C:2375:ALA:HB1	1:C:2575:TYR:CE2	2.55	0.41
1:D:3367:GLN:O	1:D:3531:THR:HG23	2.21	0.41
1:D:3488:ARG:C	1:D:3490:ALA:N	2.71	0.41
1:C:2462:PHE:O	1:C:2466:MET:HG3	2.20	0.41
1:A:451:TRP:CH2	1:A:464:GLU:HG3	2.56	0.41
1:D:3442:GLU:HB3	1:D:3443:GLY:H	1.20	0.40
1:D:3459:ALA:HA	1:D:3462:PHE:CD1	2.56	0.40
1:C:2444:ASP:OD1	1:C:2444:ASP:N	2.54	0.40
1:C:2572:TYR:HE1	1:C:2576:VAL:HG21	1.86	0.40
1:D:3473:GLU:O	1:D:3479:VAL:HB	2.21	0.40
1:C:2419:ILE:CG2	1:C:2420:GLY:N	2.83	0.40
1:D:3434:ARG:O	1:D:3438:THR:HB	2.22	0.40
1:D:3430:ALA:HB1	1:D:3435:GLU:CB	2.50	0.40
1:A:498:ASN:ND2	1:A:530:ARG:NH2	2.69	0.40
1:C:2449:ASP:OD1	1:C:2450:LEU:HG	2.21	0.40
1:C:2581:THR:HG22	1:C:2582:VAL:HG23	2.03	0.40
1:A:562:HIS:O	1:A:566:VAL:HG23	2.21	0.40
1:C:2458:PHE:HA	1:D:3439:TYR:CE2	2.56	0.40
1:B:1491:ILE:HG23	1:B:1526:LEU:HG	2.03	0.40
1:B:1358:ILE:HD13	4:B:1600:ADP:H1'	2.02	0.40
1:C:2443:GLY:O	1:C:2444:ASP:CB	2.69	0.40

There are no symmetry-related clashes.

## 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	240/243 (99%)	198 (82%)	27 (11%)	15 (6%)	2	10
1	B	240/243 (99%)	200 (83%)	29 (12%)	11 (5%)	3	17
1	C	240/243 (99%)	202 (84%)	22 (9%)	16 (7%)	1	9
1	D	239/243 (98%)	189 (79%)	34 (14%)	16 (7%)	1	9
All	All	959/972 (99%)	789 (82%)	112 (12%)	58 (6%)	2	11

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	LEU
1	A	426	SER
1	A	444	ASP
1	A	467	PRO
1	A	476	GLU
1	A	516	GLU
1	B	1347	HIS
1	B	1425	ASP
1	B	1498	ASN
1	C	2410	ILE
1	C	2426	SER
1	C	2427	ALA
1	C	2460	ARG
1	C	2467	PRO
1	C	2469	GLN
1	C	2528	LYS
1	C	2553	LYS
1	D	3354	ASP
1	D	3369	ASN
1	D	3395	PRO
1	D	3406	PRO
1	D	3408	ASP

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Mol	Chain	Res	Type
1	D	3423	SER
1	D	3426	SER
1	D	3469	GLN
1	A	513	SER
1	A	553	LYS
1	B	1439	TYR
1	B	1442	GLU
1	B	1499	PRO
1	C	2398	GLY
1	C	2425	ASP
1	C	2513	SER
1	D	3440	GLY
1	D	3508	THR
1	D	3513	SER
1	A	483	GLY
1	A	510	SER
1	A	578	GLU
1	B	1469	GLN
1	B	1480	LYS
1	C	2356	GLU
1	C	2439	TYR
1	C	2446	THR
1	D	3361	ASP
1	D	3507	ALA
1	A	458	PHE
1	B	1428	ILE
1	C	2355	SER
1	D	3347	HIS
1	D	3409	ASN
1	D	3511	LEU
1	A	361	ASP
1	A	413	GLU
1	A	425	ASP
1	B	1460	ARG
1	C	2444	ASP
1	B	1467	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	196/204 (96%)	181 (92%)	15 (8%)	16	50
1	B	202/204 (99%)	187 (93%)	15 (7%)	17	51
1	C	195/204 (96%)	183 (94%)	12 (6%)	23	59
1	D	201/204 (98%)	189 (94%)	12 (6%)	24	60
All	All	794/816 (97%)	740 (93%)	54 (7%)	20	55

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	LEU
1	A	349	ASP
1	A	408	ASP
1	A	418	GLN
1	A	421	PHE
1	A	424	GLN
1	A	448	GLU
1	A	458	PHE
1	A	461	SER
1	A	467	PRO
1	A	468	ASP
1	A	476	GLU
1	A	498	ASN
1	A	530	ARG
1	A	559	SER
1	B	1344	SER
1	B	1354	ASP
1	B	1361	ASP
1	B	1382	LYS
1	B	1391	ARG
1	B	1394	GLN
1	B	1406	PRO
1	B	1429	MET
1	B	1434	ARG
1	B	1438	THR
1	B	1446	THR
1	B	1481	ILE
1	B	1515	SER
1	B	1530	ARG
1	B	1570	PRO

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Mol	Chain	Res	Type
1	C	2343	LEU
1	C	2372	ILE
1	C	2421	PHE
1	C	2426	SER
1	C	2442	GLU
1	C	2448	GLU
1	C	2460	ARG
1	C	2467	PRO
1	C	2468	ASP
1	C	2504	LEU
1	C	2533	LEU
1	C	2572	TYR
1	D	3347	HIS
1	D	3349	ASP
1	D	3353	ASP
1	D	3368	PRO
1	D	3437	LEU
1	D	3438	THR
1	D	3442	GLU
1	D	3467	PRO
1	D	3476	GLU
1	D	3489	LEU
1	D	3513	SER
1	D	3533	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	GLN
1	A	418	GLN
1	A	498	ASN
1	B	1409	ASN
1	B	1436	ASN
1	B	1465	ASN
1	C	2394	GLN
1	C	2409	ASN
1	C	2520	GLN
1	C	2537	HIS
1	D	3405	GLN
1	D	3424	GLN
1	D	3569	HIS
1	D	3579	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 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$
3	ATP	A	601	-	24,33,33	2.35	9 (37%)	31,52,52	3.37	13 (41%)
4	ADP	B	1600	-	22,29,29	1.73	7 (31%)	27,45,45	2.51	2 (7%)
3	ATP	C	2601	-	24,33,33	2.31	9 (37%)	31,52,52	3.05	14 (45%)
4	ADP	D	3600	2	22,29,29	1.69	6 (27%)	27,45,45	2.59	1 (3%)

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
3	ATP	A	601	-	-	0/18/38/38	0/3/3/3
4	ADP	B	1600	-	-	0/12/32/32	0/3/3/3
3	ATP	C	2601	-	-	0/18/38/38	0/3/3/3
4	ADP	D	3600	2	-	0/12/32/32	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2601	ATP	O5'-C5'	-4.92	1.24	1.44
3	A	601	ATP	O5'-C5'	-3.89	1.28	1.44
3	C	2601	ATP	PA-O5'	-3.33	1.43	1.59
3	C	2601	ATP	PB-O2B	-3.28	1.40	1.54
4	D	3600	ADP	PA-O2A	-3.21	1.41	1.54
4	D	3600	ADP	PB-O3B	-3.13	1.43	1.54
4	B	1600	ADP	PA-O2A	-3.08	1.41	1.54
3	C	2601	ATP	C8-N7	-3.02	1.28	1.34
4	D	3600	ADP	PB-O1B	-3.02	1.41	1.51
4	B	1600	ADP	PB-O3B	-2.92	1.44	1.54
4	B	1600	ADP	C5-N7	-2.87	1.29	1.39
3	A	601	ATP	PA-O2A	-2.85	1.42	1.54
3	A	601	ATP	PB-O2B	-2.85	1.42	1.54
3	A	601	ATP	C8-N7	-2.84	1.29	1.34
3	C	2601	ATP	PA-O2A	-2.68	1.43	1.54
3	A	601	ATP	PA-O5'	-2.53	1.47	1.59
3	C	2601	ATP	C5-C4	-2.48	1.34	1.40
3	A	601	ATP	C3'-C4'	-2.47	1.46	1.53
4	B	1600	ADP	PB-O1B	-2.40	1.43	1.51
4	D	3600	ADP	PB-O2B	-2.30	1.46	1.54
3	C	2601	ATP	PA-O1A	-2.29	1.42	1.51
3	A	601	ATP	PB-O1B	-2.28	1.42	1.51
4	D	3600	ADP	PA-O1A	-2.26	1.42	1.51
4	B	1600	ADP	PB-O2B	-2.03	1.47	1.54
4	B	1600	ADP	O3'-C3'	2.34	1.48	1.43
4	D	3600	ADP	O4'-C1'	2.49	1.44	1.41
3	C	2601	ATP	C4-N3	2.58	1.39	1.35
4	B	1600	ADP	O4'-C1'	3.68	1.45	1.41
3	A	601	ATP	C4-N3	4.73	1.42	1.35
3	C	2601	ATP	O4'-C1'	5.49	1.48	1.41
3	A	601	ATP	O4'-C1'	5.62	1.48	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3600	ADP	N3-C2-N1	-12.55	119.29	128.89
4	B	1600	ADP	N3-C2-N1	-12.18	119.57	128.89
3	C	2601	ATP	O5'-PA-O1A	-6.44	84.60	109.62
3	A	601	ATP	O5'-PA-O1A	-6.30	85.16	109.62
3	A	601	ATP	C5'-C4'-C3'	-5.50	93.40	115.21
3	C	2601	ATP	C5'-C4'-C3'	-4.19	98.57	115.21
3	A	601	ATP	N3-C2-N1	-3.85	125.94	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2601	ATP	O3A-PA-O5'	-3.51	93.63	102.94
3	A	601	ATP	O3A-PA-O5'	-3.49	93.68	102.94
3	A	601	ATP	PA-O3A-PB	-3.43	123.11	132.73
3	C	2601	ATP	N3-C2-N1	-3.27	126.39	128.89
3	C	2601	ATP	O2A-PA-O5'	-2.56	95.54	108.46
3	A	601	ATP	C4'-O4'-C1'	-2.42	107.06	109.72
3	C	2601	ATP	C4'-O4'-C1'	-2.15	107.35	109.72
3	A	601	ATP	O4'-C4'-C5'	-2.15	101.62	109.32
3	C	2601	ATP	C1'-N9-C4	-2.15	123.70	126.94
4	B	1600	ADP	C4-C5-N7	-2.08	107.56	109.48
3	C	2601	ATP	C2'-C1'-N9	-2.06	111.14	114.29
3	C	2601	ATP	O2A-PA-O1A	2.10	123.93	112.53
3	A	601	ATP	O3'-C3'-C4'	2.44	118.36	111.05
3	C	2601	ATP	O2B-PB-O3B	2.62	116.99	105.09
3	A	601	ATP	O2B-PB-O3B	3.10	119.17	105.09
3	A	601	ATP	O2A-PA-O3A	3.41	120.58	105.09
3	C	2601	ATP	O2A-PA-O3A	3.57	121.27	105.09
3	C	2601	ATP	C4-C5-N7	4.24	113.38	109.48
3	C	2601	ATP	O4'-C4'-C3'	4.60	114.42	105.15
3	A	601	ATP	O4'-C4'-C3'	4.78	114.78	105.15
3	A	601	ATP	C4-C5-N7	5.12	114.19	109.48
3	C	2601	ATP	O5'-C5'-C4'	10.29	147.06	109.12
3	A	601	ATP	O5'-C5'-C4'	11.33	150.90	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	ATP	2	0
4	B	1600	ADP	2	0
3	C	2601	ATP	3	0
4	D	3600	ADP	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	242/243 (99%)	-0.09	13 (5%)	29 12	20, 57, 130, 176	0
1	B	242/243 (99%)	0.08	7 (2%)	55 31	26, 84, 144, 170	0
1	C	242/243 (99%)	-0.09	10 (4%)	41 19	17, 57, 126, 176	0
1	D	241/243 (99%)	0.03	9 (3%)	45 22	24, 86, 145, 153	0
All	All	967/972 (99%)	-0.01	39 (4%)	42 20	17, 67, 145, 176	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1583	GLY	6.7
1	C	2583	GLY	4.9
1	A	513	SER	4.8
1	C	2514	GLU	4.5
1	C	2508	THR	4.5
1	A	516	GLU	4.4
1	A	514	GLU	4.2
1	A	582	VAL	4.0
1	B	1479	VAL	4.0
1	A	512	ASP	3.9
1	A	426	SER	3.9
1	C	2513	SER	3.5
1	A	409	ASN	3.5
1	C	2426	SER	3.5
1	A	508	THR	3.4
1	C	2582	VAL	3.4
1	A	583	GLY	3.4
1	A	427	ALA	2.9
1	D	3422	VAL	2.8
1	D	3428	ILE	2.8
1	D	3474	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	3479	VAL	2.7
1	B	1415	TRP	2.7
1	D	3508	THR	2.7
1	C	2512	ASP	2.5
1	A	509	ALA	2.5
1	B	1445	TYR	2.5
1	B	1421	PHE	2.4
1	A	579	GLN	2.4
1	C	2581	THR	2.4
1	D	3415	TRP	2.3
1	D	3419	ILE	2.2
1	C	2509	ALA	2.2
1	B	1425	ASP	2.1
1	A	444	ASP	2.1
1	D	3343	LEU	2.1
1	C	2425	ASP	2.1
1	B	1412	LEU	2.0
1	D	3473	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ATP	A	601	31/31	0.93	0.18	0.63	49,57,97,99	0
3	ATP	C	2601	31/31	0.95	0.18	0.50	37,52,89,95	0
4	ADP	B	1600	27/27	0.97	0.16	-0.36	19,42,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ADP	D	3600	27/27	0.97	0.14	-0.67	17,37,50,52	0
2	MG	C	1601	1/1	0.89	0.31	-	76,76,76,76	0
2	MG	D	3601	1/1	0.95	0.15	-	36,36,36,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.