



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:29 PM GMT

PDB ID : 1XDP  
Title : Crystal Structure of the E.coli Polyphosphate Kinase in complex with AMPPNP  
Authors : Zhu, Y.; Huang, W.; Lee, S.S.; Xu, W.  
Deposited on : 2004-09-07  
Resolution : 2.50 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

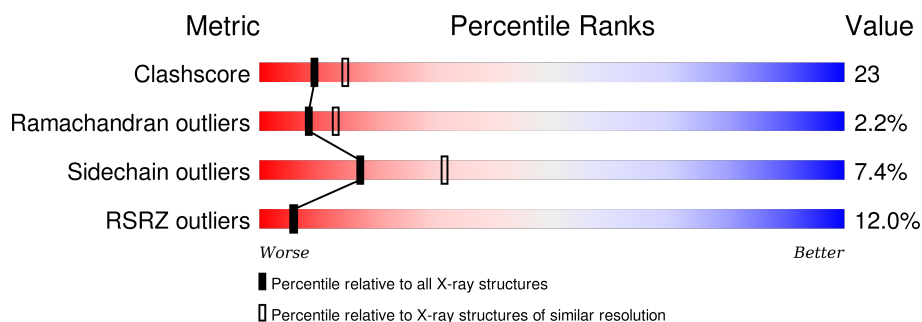
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	687	<div> <div>12%</div> <div>58%</div> <div>37%</div> <div>.</div> </div>
1	B	687	<div> <div>12%</div> <div>57%</div> <div>39%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	A	701	-	-	-	X
3	ATP	B	704	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11538 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.

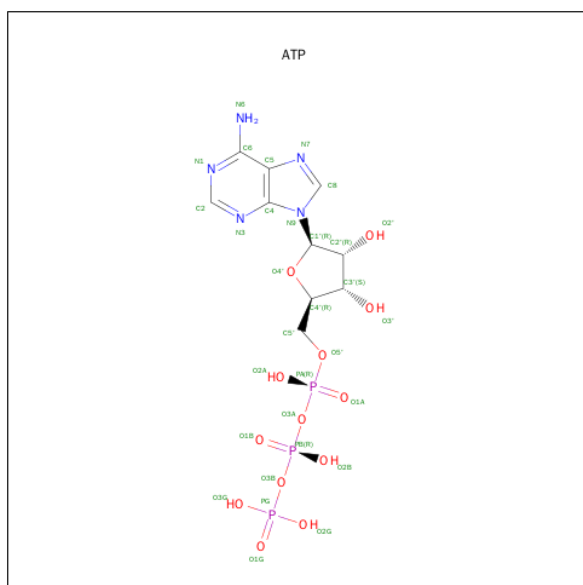
- Molecule 1 is a protein called Polyphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	0	0
			5671	3621	1008	1026	16			
1	B	687	Total	C	N	O	S	0	0	0
			5671	3621	1008	1026	16			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total	O	0	0
			76	76		
4	B	54	Total	O	0	0
			54	54		

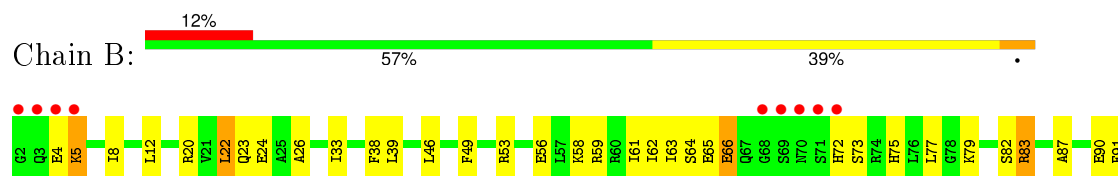
### 3 Residue-property plots

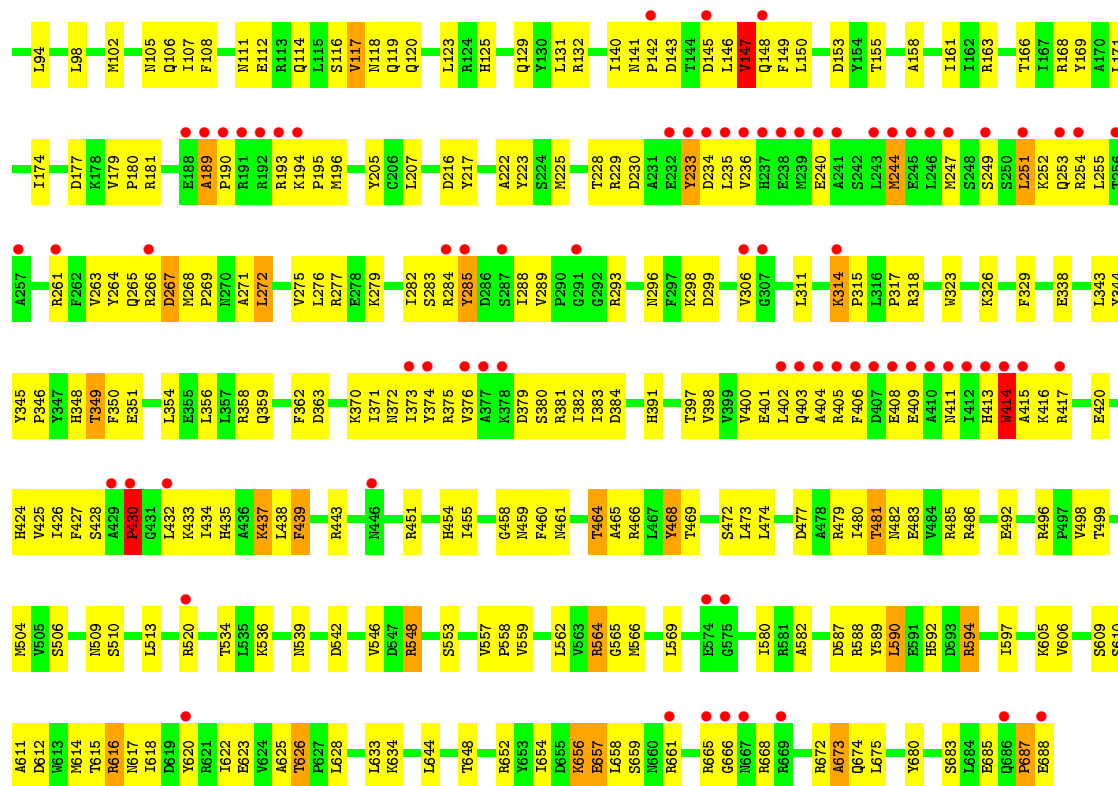
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Polyphosphate kinase



#### • Molecule 1: Polyphosphate kinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.00Å 152.00Å 150.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.96 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 97.3 (19.96-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.248 , 0.274 0.258 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.5	EDS
Estimated twinning fraction	0.025 for -h,-l,-k 0.008 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 60358 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	11538	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.42	0/5789	0.74	3/7825 (0.0%)
1	B	0.41	0/5789	0.74	4/7825 (0.1%)
All	All	0.41	0/11578	0.74	7/15650 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	594	ARG	NE-CZ-NH2	20.15	130.37	120.30
1	B	594	ARG	NE-CZ-NH1	19.79	130.19	120.30
1	A	594	ARG	NE-CZ-NH1	-12.96	113.82	120.30
1	B	594	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	A	594	ARG	CD-NE-CZ	11.10	139.14	123.60
1	B	594	ARG	CD-NE-CZ	9.13	136.38	123.60
1	B	594	ARG	CG-CD-NE	6.37	125.17	111.80

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	5671	0	5721	256	0
1	B	5671	0	5721	265	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	31	0	12	2	0
3	B	31	0	12	6	0
4	A	76	0	0	3	0
4	B	54	0	0	6	0
All	All	11538	0	11466	517	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 23.

All (517) 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:66:GLU:HG3	1:A:251:LEU:HG	1.43	1.00
1:B:672:ARG:HD3	1:B:675:LEU:HD12	1.39	1.00
1:A:672:ARG:HD3	1:A:675:LEU:HD12	1.43	0.99
1:B:66:GLU:HG3	1:B:251:LEU:HG	1.45	0.99
1:A:193:ARG:HB3	1:A:195:PRO:HD3	1.54	0.90
1:A:277:ARG:HG2	1:A:282:ILE:HD12	1.54	0.88
1:B:193:ARG:HB3	1:B:195:PRO:HD3	1.54	0.88
1:B:277:ARG:HG2	1:B:282:ILE:HD12	1.56	0.87
1:A:435:HIS:NE2	3:A:701:ATP:O3G	2.09	0.85
1:B:240:GLU:HB3	1:B:244:MET:HB2	1.60	0.84
1:A:63:ILE:HG12	1:A:255:LEU:HD11	1.60	0.83
1:A:240:GLU:HB3	1:A:244:MET:HB2	1.60	0.83
1:B:179:VAL:HG13	1:B:180:PRO:HD2	1.61	0.81
1:A:426:ILE:HD13	1:A:492:GLU:HG2	1.63	0.81
1:B:63:ILE:HG12	1:B:255:LEU:HD11	1.60	0.81
1:A:402:LEU:HD22	1:A:427:PHE:HD2	1.43	0.81
1:B:402:LEU:HD22	1:B:427:PHE:HD2	1.46	0.81
1:A:141:ASN:HB3	1:A:142:PRO:HD2	1.63	0.81
1:B:141:ASN:HB3	1:B:142:PRO:HD2	1.63	0.80
1:A:344:TYR:H	1:A:348:HIS:HD2	1.25	0.80
1:B:344:TYR:H	1:B:348:HIS:HD2	1.28	0.79
1:A:179:VAL:HG13	1:A:180:PRO:HD2	1.65	0.79
1:B:426:ILE:HD13	1:B:492:GLU:HG2	1.65	0.78
3:B:704:ATP:H2'	3:B:704:ATP:N3	1.99	0.77
1:A:53:ARG:HH12	1:A:566:MET:HE2	1.50	0.77
1:B:244:MET:HA	1:B:247:MET:HB2	1.67	0.76
1:A:614:MET:HB2	1:A:617:ASN:ND2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:MET:HB2	1:B:617:ASN:ND2	2.00	0.76
1:B:403:GLN:HE22	1:B:430:PRO:HA	1.51	0.76
1:A:244:MET:HA	1:A:247:MET:HB2	1.68	0.76
1:B:413:HIS:C	1:B:415:ALA:H	1.89	0.76
1:B:116:SER:C	1:B:118:ASN:H	1.89	0.75
1:A:116:SER:C	1:A:118:ASN:H	1.89	0.75
1:A:594:ARG:HH21	1:A:610:SER:C	1.89	0.75
1:B:594:ARG:HD3	1:B:612:ASP:OD1	1.87	0.75
1:A:413:HIS:C	1:A:415:ALA:H	1.89	0.74
1:A:403:GLN:HE22	1:A:430:PRO:HA	1.52	0.74
1:A:111:ASN:H	1:A:114:GLN:HE21	1.36	0.74
1:A:61:ILE:HD13	1:A:73:SER:HB2	1.70	0.73
1:A:20:ARG:HG2	1:A:652:ARG:HD2	1.70	0.72
1:A:265:GLN:HE21	1:A:293:ARG:HA	1.53	0.72
1:B:111:ASN:H	1:B:114:GLN:HE21	1.37	0.72
1:B:61:ILE:HD13	1:B:73:SER:HB2	1.70	0.72
1:B:468:TYR:OH	3:B:704:ATP:O3'	2.08	0.72
1:B:20:ARG:HG2	1:B:652:ARG:HD2	1.70	0.72
1:A:22:LEU:HD22	1:A:94:LEU:HD12	1.71	0.71
1:B:437:LYS:HG2	1:B:458:GLY:O	1.89	0.71
1:B:265:GLN:HE21	1:B:293:ARG:HA	1.54	0.71
1:A:437:LYS:HG2	1:A:458:GLY:O	1.91	0.71
1:B:22:LEU:HD22	1:B:94:LEU:HD12	1.71	0.70
1:B:606:VAL:HG21	1:B:634:LYS:HG3	1.72	0.70
1:A:240:GLU:CB	1:A:244:MET:HB2	2.22	0.70
1:A:345:TYR:O	1:A:469:THR:HA	1.92	0.70
1:B:106:GLN:O	1:B:194:LYS:HB2	1.92	0.69
1:A:163:ARG:O	1:A:166:THR:HB	1.92	0.69
1:B:163:ARG:O	1:B:166:THR:HB	1.94	0.68
1:A:426:ILE:CD1	1:A:492:GLU:HG2	2.23	0.68
1:A:380:SER:HB3	1:A:383:ILE:HG12	1.77	0.67
1:B:33:ILE:HG12	1:B:311:LEU:HB3	1.76	0.67
1:A:106:GLN:O	1:A:194:LYS:HB2	1.95	0.67
1:B:240:GLU:CB	1:B:244:MET:HB2	2.22	0.67
1:B:265:GLN:NE2	1:B:293:ARG:HG3	2.10	0.67
1:A:265:GLN:NE2	1:A:293:ARG:HG3	2.09	0.67
1:B:288:ILE:HD12	1:B:288:ILE:N	2.10	0.67
1:A:370:LYS:HG2	1:A:397:THR:HB	1.77	0.67
1:B:53:ARG:HH12	1:B:566:MET:HE2	1.58	0.67
1:B:426:ILE:CD1	1:B:492:GLU:HG2	2.25	0.67
1:A:72:HIS:HB3	1:A:75:HIS:CD2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:HG12	1:A:311:LEU:HB3	1.76	0.66
1:B:72:HIS:HB3	1:B:75:HIS:CD2	2.31	0.66
1:A:139:LEU:HD11	1:B:362:PHE:O	1.96	0.66
1:B:370:LYS:HG2	1:B:397:THR:HB	1.78	0.65
1:B:59:ARG:O	1:B:63:ILE:HG13	1.97	0.65
1:A:288:ILE:N	1:A:288:ILE:HD12	2.12	0.65
1:B:23:GLN:OE1	1:B:652:ARG:HD3	1.97	0.65
1:B:345:TYR:O	1:B:469:THR:HA	1.96	0.65
1:A:59:ARG:O	1:A:63:ILE:HG13	1.96	0.65
1:A:53:ARG:NH1	1:A:566:MET:HE2	2.12	0.64
1:A:363:ASP:OD2	1:A:443:ARG:NH1	2.30	0.64
1:A:53:ARG:NH1	1:A:566:MET:CE	2.59	0.64
1:B:380:SER:HB3	1:B:383:ILE:HG12	1.78	0.64
1:A:23:GLN:OE1	1:A:652:ARG:HD3	1.98	0.64
1:B:582:ALA:HB1	1:B:654:ILE:HD12	1.80	0.64
1:B:155:THR:O	1:B:174:ILE:HG12	1.98	0.64
1:A:149:PHE:HB3	1:B:391:HIS:CE1	2.33	0.63
1:A:214:PHE:HZ	1:B:359:GLN:OE1	1.82	0.63
1:B:416:LYS:O	1:B:420:GLU:HB2	1.97	0.63
1:A:416:LYS:O	1:A:420:GLU:HB2	1.97	0.63
1:B:559:VAL:HB	1:B:580:ILE:HG12	1.81	0.63
1:A:614:MET:HB2	1:A:617:ASN:HD22	1.62	0.63
1:B:614:MET:HB2	1:B:617:ASN:HD22	1.62	0.63
1:A:155:THR:O	1:A:174:ILE:HG12	1.99	0.62
1:B:189:ALA:HB3	1:B:190:PRO:CD	2.28	0.62
1:A:413:HIS:ND1	1:A:416:LYS:HE3	2.14	0.62
1:B:363:ASP:OD2	1:B:443:ARG:NH1	2.32	0.62
1:A:189:ALA:HB3	1:A:190:PRO:CD	2.29	0.62
1:A:480:ILE:HD12	4:A:771:HOH:O	1.98	0.62
1:A:75:HIS:O	1:A:79:LYS:HG3	2.00	0.62
1:A:435:HIS:HE2	3:A:701:ATP:PG	2.22	0.62
1:A:548:ARG:HG2	1:A:548:ARG:HH11	1.64	0.61
1:B:75:HIS:O	1:B:79:LYS:HG3	2.00	0.61
1:A:322:ILE:HG23	4:A:753:HOH:O	2.00	0.61
1:A:606:VAL:HG21	1:A:634:LYS:HG3	1.80	0.61
1:B:371:ILE:HG13	1:B:439:PHE:HB3	1.83	0.61
1:A:207:LEU:HD11	1:A:222:ALA:HB2	1.82	0.61
1:A:559:VAL:HB	1:A:580:ILE:HG12	1.81	0.61
1:B:207:LEU:HD11	1:B:222:ALA:HB2	1.81	0.61
1:B:413:HIS:ND1	1:B:416:LYS:HE3	2.16	0.61
1:A:401:GLU:OE2	1:A:403:GLN:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:LYS:HG3	1:B:657:GLU:OE1	2.00	0.60
1:B:401:GLU:OE2	1:B:403:GLN:HB2	2.01	0.60
1:B:606:VAL:CG2	1:B:634:LYS:HG3	2.31	0.60
1:B:504:MET:HB3	1:B:625:ALA:HB3	1.82	0.60
1:B:83:ARG:HG2	1:B:83:ARG:HH11	1.65	0.60
1:A:582:ALA:HB1	1:A:654:ILE:HD12	1.84	0.60
1:B:548:ARG:HG2	1:B:548:ARG:HH11	1.67	0.60
1:A:504:MET:HB3	1:A:625:ALA:HB3	1.83	0.60
1:B:72:HIS:HB3	1:B:75:HIS:HD2	1.67	0.60
1:A:72:HIS:HB3	1:A:75:HIS:HD2	1.67	0.59
1:A:111:ASN:H	1:A:114:GLN:NE2	1.99	0.59
1:B:53:ARG:NH1	1:B:566:MET:CE	2.64	0.59
1:B:373:ILE:HG23	1:B:376:VAL:HG13	1.83	0.59
1:A:594:ARG:NH2	1:A:610:SER:O	2.34	0.59
1:A:373:ILE:HG23	1:A:376:VAL:HG13	1.84	0.59
1:B:116:SER:O	1:B:120:GLN:HG3	2.03	0.59
1:B:147:VAL:HG22	1:B:279:LYS:O	2.03	0.59
1:B:536:LYS:HD3	1:B:562:LEU:HD23	1.85	0.59
1:B:111:ASN:H	1:B:114:GLN:NE2	2.01	0.59
1:A:116:SER:OG	1:A:119:GLN:HG3	2.03	0.59
1:A:656:LYS:HG3	1:A:657:GLU:OE1	2.03	0.58
1:B:26:ALA:HB2	1:B:94:LEU:HD11	1.85	0.58
1:B:594:ARG:NH2	1:B:610:SER:O	2.35	0.58
1:B:116:SER:O	1:B:118:ASN:N	2.37	0.58
1:B:376:VAL:HG23	1:B:414:TRP:HE1	1.67	0.58
1:A:323:TRP:HZ2	1:A:338:GLU:HG2	1.68	0.58
1:B:112:GLU:HB2	1:B:205:TYR:HB2	1.84	0.58
1:A:26:ALA:HB2	1:A:94:LEU:HD11	1.86	0.58
1:B:633:LEU:HD12	4:B:714:HOH:O	2.04	0.58
1:B:314:LYS:H	1:B:314:LYS:HD3	1.68	0.58
1:B:116:SER:OG	1:B:119:GLN:HG3	2.03	0.57
1:B:432:LEU:HD22	1:B:620:TYR:O	2.05	0.57
1:A:506:SER:O	1:A:622:ILE:HA	2.04	0.57
1:A:116:SER:O	1:A:120:GLN:HG3	2.04	0.57
1:A:314:LYS:H	1:A:314:LYS:HD3	1.67	0.57
1:A:432:LEU:HD22	1:A:620:TYR:O	2.05	0.57
1:A:116:SER:O	1:A:118:ASN:N	2.37	0.57
1:B:374:TYR:O	1:B:411:ASN:ND2	2.36	0.57
1:A:413:HIS:C	1:A:415:ALA:N	2.58	0.57
1:A:147:VAL:HG22	1:A:279:LYS:O	2.04	0.57
1:B:408:GLU:HG3	1:B:409:GLU:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:VAL:HG23	1:A:414:TRP:HE1	1.67	0.57
1:A:112:GLU:OE1	1:A:293:ARG:NH2	2.35	0.57
1:A:371:ILE:HG13	1:A:439:PHE:HB3	1.87	0.57
1:B:461:ASN:HB3	1:B:464:THR:HB	1.87	0.57
1:B:323:TRP:HZ2	1:B:338:GLU:HG2	1.70	0.56
1:A:140:ILE:HD11	1:A:171:LEU:HG	1.86	0.56
1:A:408:GLU:HG3	1:A:409:GLU:N	2.20	0.56
1:A:112:GLU:HB2	1:A:205:TYR:HB2	1.87	0.56
1:A:265:GLN:HE22	1:A:293:ARG:HG3	1.70	0.56
1:A:461:ASN:HB3	1:A:464:THR:HB	1.87	0.56
1:A:56:GLU:HA	1:A:59:ARG:NH1	2.20	0.56
1:A:536:LYS:HD3	1:A:562:LEU:HD23	1.87	0.56
1:A:223:TYR:HA	1:A:265:GLN:OE1	2.05	0.56
1:A:374:TYR:O	1:A:411:ASN:ND2	2.38	0.56
1:B:140:ILE:HD11	1:B:171:LEU:HG	1.87	0.56
1:B:348:HIS:HE1	1:B:685:GLU:OE1	1.88	0.56
1:B:53:ARG:NH1	1:B:566:MET:HE2	2.21	0.56
1:B:509:ASN:ND2	1:B:513:LEU:HD22	2.21	0.56
1:A:59:ARG:HD3	1:A:255:LEU:O	2.06	0.56
1:B:506:SER:O	1:B:622:ILE:HA	2.06	0.55
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.69	0.55
1:A:401:GLU:OE1	1:A:428:SER:HB2	2.07	0.55
1:B:112:GLU:OE1	1:B:293:ARG:NH2	2.36	0.55
1:B:56:GLU:HA	1:B:59:ARG:NH1	2.20	0.55
1:B:401:GLU:OE1	1:B:428:SER:HB2	2.07	0.55
1:A:348:HIS:HE1	1:A:685:GLU:OE1	1.90	0.55
1:B:39:LEU:HD22	1:B:91:PHE:CE1	2.42	0.54
1:B:265:GLN:HE21	1:B:293:ARG:CA	2.20	0.54
1:A:265:GLN:HE21	1:A:293:ARG:CA	2.21	0.54
1:A:432:LEU:HD11	1:A:622:ILE:HG13	1.89	0.54
1:A:538:ASN:ND2	1:A:594:ARG:HH11	2.05	0.54
1:A:116:SER:C	1:A:118:ASN:N	2.58	0.54
1:A:414:TRP:CE3	1:A:414:TRP:HA	2.42	0.54
1:A:323:TRP:CZ2	1:A:338:GLU:HG2	2.42	0.54
1:B:39:LEU:HD11	1:B:98:LEU:HD12	1.90	0.54
1:B:455:ILE:HG21	1:B:626:THR:OG1	2.07	0.54
1:B:451:ARG:HB2	1:B:481:THR:CG2	2.37	0.54
1:B:225:MET:HE1	1:B:276:LEU:HD13	1.90	0.54
1:B:520:ARG:HH11	1:B:605:LYS:HZ3	1.55	0.54
1:B:223:TYR:HA	1:B:265:GLN:OE1	2.08	0.54
1:A:451:ARG:HB2	1:A:481:THR:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:CG	1:A:251:LEU:HG	2.28	0.53
1:B:59:ARG:HH11	1:B:236:VAL:HG21	1.72	0.53
1:B:432:LEU:HD11	1:B:622:ILE:HG13	1.90	0.53
1:B:265:GLN:HE22	1:B:293:ARG:HG3	1.71	0.53
1:A:120:GLN:HB3	1:A:205:TYR:OH	2.09	0.53
1:B:59:ARG:HD3	1:B:255:LEU:O	2.06	0.53
1:B:263:VAL:HA	1:B:289:VAL:O	2.09	0.53
1:B:644:LEU:HD23	1:B:673:ALA:HB1	1.91	0.53
1:B:592:HIS:CE1	1:B:594:ARG:HH12	2.26	0.53
1:A:414:TRP:HE3	1:A:414:TRP:HA	1.73	0.53
1:B:414:TRP:CE3	1:B:414:TRP:HA	2.43	0.53
1:B:414:TRP:HE3	1:B:414:TRP:HA	1.74	0.53
1:A:425:VAL:HG12	1:A:426:ILE:N	2.24	0.53
1:A:644:LEU:HD23	1:A:673:ALA:HB1	1.90	0.53
1:B:117:VAL:HG12	1:B:117:VAL:O	2.09	0.53
1:A:455:ILE:HG21	1:A:626:THR:OG1	2.09	0.53
1:B:271:ALA:O	1:B:275:VAL:HG23	2.08	0.53
1:A:22:LEU:CD2	1:A:94:LEU:HD12	2.39	0.53
1:A:509:ASN:ND2	1:A:513:LEU:HD22	2.23	0.53
1:A:468:TYR:N	1:A:468:TYR:CD1	2.77	0.53
1:A:39:LEU:HD22	1:A:91:PHE:CE1	2.43	0.53
1:B:382:ILE:CD1	1:B:460:PHE:HB3	2.39	0.53
1:B:408:GLU:HG3	1:B:409:GLU:H	1.74	0.52
1:A:117:VAL:HG12	1:A:117:VAL:O	2.09	0.52
1:B:22:LEU:CD2	1:B:94:LEU:HD12	2.38	0.52
1:A:468:TYR:N	1:A:468:TYR:HD1	2.07	0.52
1:A:263:VAL:HA	1:A:289:VAL:O	2.09	0.52
1:A:315:PRO:O	1:A:317:PRO:HD3	2.09	0.52
1:B:181:ARG:HD2	1:B:299:ASP:OD2	2.10	0.52
1:B:24:GLU:HB3	1:B:38:PHE:CE1	2.43	0.52
1:B:688:GLU:HG3	4:B:754:HOH:O	2.08	0.52
1:A:59:ARG:HH11	1:A:236:VAL:HG21	1.72	0.52
1:B:265:GLN:NE2	1:B:293:ARG:HA	2.22	0.52
1:A:606:VAL:CG2	1:A:634:LYS:HG3	2.38	0.52
1:B:509:ASN:HD22	1:B:513:LEU:HD22	1.74	0.52
1:B:277:ARG:HA	1:B:282:ILE:HD12	1.92	0.52
1:A:163:ARG:HG3	1:A:216:ASP:O	2.09	0.52
1:B:163:ARG:HG3	1:B:216:ASP:O	2.09	0.52
1:A:149:PHE:CB	1:B:391:HIS:CE1	2.93	0.52
1:B:323:TRP:CZ2	1:B:338:GLU:HG2	2.44	0.52
1:A:56:GLU:HA	1:A:59:ARG:HH12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ARG:NH2	4:B:739:HOH:O	2.43	0.51
1:B:116:SER:C	1:B:118:ASN:N	2.58	0.51
1:B:79:LYS:O	1:B:82:SER:HB3	2.09	0.51
1:B:379:ASP:HA	1:B:414:TRP:CH2	2.46	0.51
1:A:8:ILE:HD13	1:A:658:LEU:HD21	1.91	0.51
1:B:483:GLU:OE2	1:B:486:ARG:NH2	2.44	0.51
1:A:194:LYS:HB3	1:A:306:VAL:HG11	1.92	0.51
1:A:408:GLU:HG3	1:A:409:GLU:H	1.74	0.51
1:B:468:TYR:N	1:B:468:TYR:HD1	2.09	0.51
1:A:382:ILE:CD1	1:A:460:PHE:HB3	2.40	0.51
1:A:277:ARG:HA	1:A:282:ILE:HD12	1.93	0.51
1:B:282:ILE:HG21	1:B:288:ILE:HD11	1.93	0.51
1:A:435:HIS:HB3	1:A:623:GLU:OE1	2.10	0.51
1:B:425:VAL:HG12	1:B:426:ILE:N	2.25	0.51
1:B:413:HIS:C	1:B:415:ALA:N	2.58	0.51
1:B:480:ILE:HD12	4:B:730:HOH:O	2.11	0.51
1:B:468:TYR:CD1	1:B:468:TYR:N	2.78	0.51
1:A:145:ASP:HB2	1:A:147:VAL:HG23	1.92	0.51
1:A:61:ILE:O	1:A:65:GLU:HG3	2.11	0.51
1:B:163:ARG:HG2	1:B:217:TYR:HA	1.93	0.51
1:B:120:GLN:HB3	1:B:205:TYR:OH	2.11	0.50
1:A:553:SER:HB2	1:A:580:ILE:HG13	1.93	0.50
1:A:108:PHE:CZ	1:A:193:ARG:NH1	2.79	0.50
1:A:282:ILE:HG21	1:A:288:ILE:HD11	1.93	0.50
1:A:79:LYS:O	1:A:82:SER:HB3	2.10	0.50
1:B:145:ASP:HB2	1:B:147:VAL:HG23	1.93	0.50
1:B:56:GLU:HA	1:B:59:ARG:HH12	1.75	0.50
1:B:194:LYS:HB3	1:B:306:VAL:HG11	1.92	0.50
1:B:22:LEU:HD22	1:B:94:LEU:CD1	2.41	0.50
1:B:553:SER:HB2	1:B:580:ILE:HG13	1.93	0.50
1:B:8:ILE:HD13	1:B:658:LEU:HD21	1.92	0.50
1:A:379:ASP:HA	1:A:414:TRP:CH2	2.47	0.50
1:A:657:GLU:OE1	1:A:657:GLU:N	2.42	0.50
1:B:454:HIS:HA	1:B:473:LEU:O	2.12	0.50
1:B:402:LEU:HD22	1:B:427:PHE:CD2	2.37	0.50
1:B:20:ARG:CG	1:B:652:ARG:HD2	2.41	0.50
1:A:24:GLU:HB3	1:A:38:PHE:CE1	2.46	0.50
1:B:267:ASP:O	1:B:268:MET:C	2.50	0.50
1:B:589:TYR:HB2	1:B:674:GLN:NE2	2.27	0.50
1:B:594:ARG:HB2	1:B:609:SER:O	2.12	0.50
1:B:504:MET:HG3	1:B:513:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:TYR:HD1	1:A:285:TYR:H	1.58	0.50
1:B:315:PRO:O	1:B:317:PRO:HD3	2.11	0.50
1:A:454:HIS:HA	1:A:473:LEU:O	2.12	0.50
1:B:108:PHE:CZ	1:B:193:ARG:NH1	2.80	0.50
1:B:437:LYS:HG2	1:B:458:GLY:C	2.32	0.50
1:B:59:ARG:HB3	1:B:255:LEU:HD22	1.94	0.49
1:B:665:ARG:HG3	1:B:665:ARG:O	2.10	0.49
1:A:589:TYR:HB2	1:A:674:GLN:NE2	2.27	0.49
1:A:225:MET:HE1	1:A:276:LEU:HD13	1.94	0.49
1:B:66:GLU:CG	1:B:251:LEU:HG	2.29	0.49
1:B:83:ARG:HD2	1:B:83:ARG:H	1.77	0.49
1:B:228:THR:HG22	1:B:229:ARG:N	2.26	0.49
1:B:468:TYR:HH	3:B:704:ATP:HO3'	1.52	0.49
1:A:265:GLN:NE2	1:A:293:ARG:HA	2.22	0.49
1:B:61:ILE:O	1:B:65:GLU:HG3	2.12	0.49
1:A:163:ARG:HG2	1:A:217:TYR:HA	1.93	0.49
1:A:39:LEU:HD11	1:A:98:LEU:HD12	1.93	0.49
1:B:189:ALA:HB3	1:B:190:PRO:HD3	1.94	0.49
1:B:288:ILE:HD12	1:B:288:ILE:H	1.77	0.49
1:A:251:LEU:O	1:A:255:LEU:HB2	2.13	0.49
1:A:181:ARG:HD2	1:A:299:ASP:OD2	2.11	0.49
1:A:228:THR:HG22	1:A:229:ARG:N	2.26	0.49
1:A:59:ARG:HB3	1:A:255:LEU:HD22	1.93	0.49
1:B:314:LYS:H	1:B:314:LYS:CD	2.24	0.49
1:B:285:TYR:H	1:B:285:TYR:HD1	1.59	0.49
1:A:271:ALA:O	1:A:275:VAL:HG23	2.12	0.49
1:A:665:ARG:HG3	1:A:665:ARG:O	2.10	0.49
1:B:251:LEU:O	1:B:255:LEU:HB2	2.13	0.49
1:A:267:ASP:O	1:A:268:MET:C	2.50	0.49
1:A:4:GLU:O	1:A:5:LYS:C	2.51	0.48
1:A:251:LEU:CD2	1:A:255:LEU:HG	2.43	0.48
1:B:569:LEU:HD23	1:B:569:LEU:C	2.34	0.48
1:B:251:LEU:CD2	1:B:255:LEU:HG	2.43	0.48
1:A:77:LEU:HD22	1:A:77:LEU:N	2.28	0.48
1:B:468:TYR:OH	3:B:704:ATP:H3'	2.13	0.48
1:A:22:LEU:HD22	1:A:94:LEU:CD1	2.42	0.48
1:B:657:GLU:N	1:B:657:GLU:OE1	2.44	0.48
1:B:4:GLU:O	1:B:5:LYS:C	2.51	0.48
1:B:435:HIS:HB3	1:B:623:GLU:OE1	2.14	0.48
1:A:504:MET:HG3	1:A:513:LEU:HD23	1.96	0.48
1:B:77:LEU:N	1:B:77:LEU:HD22	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LYS:HE3	1:A:459:ASN:HB3	1.96	0.48
1:B:169:TYR:CE2	1:B:272:LEU:HG	2.48	0.48
1:A:169:TYR:CE2	1:A:272:LEU:HG	2.49	0.48
1:A:20:ARG:CG	1:A:652:ARG:HD2	2.42	0.48
1:A:402:LEU:HD22	1:A:427:PHE:CD2	2.35	0.47
1:A:537:LEU:HA	1:A:594:ARG:HG2	1.96	0.47
1:A:509:ASN:HD22	1:A:513:LEU:HD22	1.78	0.47
1:B:539:ASN:ND2	1:B:566:MET:H	2.12	0.47
1:A:538:ASN:HD22	1:A:594:ARG:HH11	1.62	0.47
1:A:536:LYS:O	1:A:594:ARG:HA	2.15	0.47
1:A:111:ASN:N	1:A:114:GLN:HE21	2.10	0.47
1:A:314:LYS:H	1:A:314:LYS:CD	2.24	0.47
1:A:539:ASN:ND2	1:A:566:MET:H	2.13	0.47
1:A:105:ASN:O	1:A:106:GLN:HB2	2.14	0.47
1:B:179:VAL:HG13	1:B:180:PRO:CD	2.39	0.47
1:A:189:ALA:HB3	1:A:190:PRO:HD3	1.96	0.47
1:B:105:ASN:O	1:B:106:GLN:HB2	2.14	0.47
1:B:179:VAL:CG1	1:B:180:PRO:HD2	2.39	0.47
1:B:102:MET:HB3	1:B:107:ILE:HB	1.96	0.47
1:B:20:ARG:NH2	4:B:750:HOH:O	2.47	0.47
1:A:288:ILE:H	1:A:288:ILE:HD12	1.79	0.47
1:A:659:SER:OG	1:A:661:ARG:HG3	2.15	0.47
1:A:498:VAL:HG12	1:A:499:THR:N	2.29	0.47
1:A:539:ASN:HD22	1:A:566:MET:H	1.63	0.47
1:A:116:SER:HG	1:A:119:GLN:HG3	1.78	0.46
1:A:161:ILE:HB	1:A:168:ARG:HB2	1.96	0.46
1:A:61:ILE:CD1	1:A:77:LEU:HD21	2.46	0.46
1:B:145:ASP:CG	1:B:145:ASP:O	2.54	0.46
1:B:564:ARG:HG3	1:B:565:GLY:N	2.30	0.46
1:A:413:HIS:O	1:A:415:ALA:N	2.47	0.46
1:A:77:LEU:H	1:A:77:LEU:HD22	1.80	0.46
1:A:284:ARG:HG3	1:A:285:TYR:N	2.30	0.46
1:B:225:MET:CE	1:B:276:LEU:HD13	2.46	0.46
1:A:680:TYR:O	1:A:683:SER:HB3	2.16	0.46
1:A:225:MET:CE	1:A:276:LEU:HD13	2.46	0.46
1:A:483:GLU:OE2	1:A:486:ARG:NH2	2.48	0.46
1:B:161:ILE:HB	1:B:168:ARG:HB2	1.98	0.46
1:A:437:LYS:HG2	1:A:458:GLY:C	2.35	0.46
1:B:400:VAL:O	1:B:400:VAL:HG23	2.16	0.46
1:A:411:ASN:HA	1:A:414:TRP:HB2	1.98	0.46
1:A:400:VAL:HG23	1:A:400:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:ARG:HH21	1:B:610:SER:C	2.19	0.46
1:B:451:ARG:HB2	1:B:481:THR:HG21	1.96	0.46
1:B:284:ARG:HG3	1:B:285:TYR:N	2.31	0.45
1:A:350:PHE:HB2	1:A:465:ALA:HB1	1.98	0.45
1:B:498:VAL:HG12	1:B:499:THR:N	2.31	0.45
1:A:235:LEU:HD21	1:A:433:LYS:NZ	2.31	0.45
1:A:63:ILE:HG13	1:A:255:LEU:HD21	1.97	0.45
1:B:63:ILE:HG13	1:B:255:LEU:HD21	1.97	0.45
1:B:413:HIS:O	1:B:415:ALA:N	2.48	0.45
1:A:451:ARG:HB2	1:A:481:THR:HG21	1.97	0.45
1:A:355:GLU:HG2	1:B:132:ARG:NH1	2.31	0.45
1:A:542:ASP:O	1:A:546:VAL:HG23	2.16	0.45
1:B:63:ILE:CG1	1:B:255:LEU:HD11	2.40	0.45
1:B:373:ILE:HG23	1:B:376:VAL:CG1	2.46	0.45
1:A:145:ASP:CG	1:A:145:ASP:O	2.54	0.45
1:B:194:LYS:N	1:B:195:PRO:CD	2.79	0.45
1:B:437:LYS:HG3	1:B:459:ASN:HA	1.97	0.45
1:B:61:ILE:CD1	1:B:77:LEU:HD21	2.46	0.45
1:B:77:LEU:HD22	1:B:77:LEU:H	1.81	0.45
1:A:323:TRP:CZ2	1:A:329:PHE:HZ	2.34	0.45
1:B:326:LYS:HE2	1:B:688:GLU:OE2	2.16	0.45
1:A:435:HIS:O	1:A:437:LYS:HD2	2.16	0.45
1:A:83:ARG:HD2	1:A:83:ARG:H	1.81	0.45
1:A:437:LYS:HG3	1:A:459:ASN:HA	1.98	0.45
1:A:179:VAL:HG13	1:A:180:PRO:CD	2.42	0.45
1:A:577:SER:HB2	1:A:580:ILE:HD12	1.98	0.45
1:A:615:THR:HG22	1:A:620:TYR:HE1	1.82	0.45
1:B:190:PRO:HG2	1:B:193:ARG:HD3	1.99	0.45
1:B:539:ASN:HD22	1:B:566:MET:H	1.63	0.45
1:A:12:LEU:HD11	1:A:79:LYS:HD2	1.98	0.45
1:A:482:ASN:O	1:A:485:ARG:HB3	2.16	0.45
1:B:59:ARG:HB3	1:B:255:LEU:CD2	2.47	0.45
1:B:439:PHE:C	1:B:439:PHE:CD1	2.90	0.45
1:B:411:ASN:HA	1:B:414:TRP:HB2	1.98	0.45
1:A:194:LYS:N	1:A:195:PRO:CD	2.80	0.44
1:A:225:MET:HE1	1:A:276:LEU:HD22	1.99	0.44
1:B:587:ASP:CG	1:B:588:ARG:H	2.19	0.44
1:A:59:ARG:HB3	1:A:255:LEU:CD2	2.46	0.44
1:A:63:ILE:CG1	1:A:255:LEU:HD11	2.39	0.44
1:B:116:SER:HG	1:B:119:GLN:HG3	1.81	0.44
1:A:79:LYS:O	1:A:83:ARG:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:PHE:HB2	1:B:465:ALA:HB1	1.99	0.44
1:B:680:TYR:O	1:B:683:SER:HB3	2.16	0.44
1:B:437:LYS:HE3	1:B:459:ASN:HB3	2.00	0.44
1:B:468:TYR:OH	3:B:704:ATP:C3'	2.66	0.44
1:A:439:PHE:CD1	1:A:439:PHE:C	2.91	0.44
1:B:482:ASN:O	1:B:485:ARG:HB3	2.17	0.44
1:B:564:ARG:CZ	1:B:590:LEU:HD21	2.48	0.44
1:A:344:TYR:H	1:A:348:HIS:CD2	2.16	0.44
1:A:131:LEU:O	1:A:132:ARG:C	2.56	0.44
1:B:354:LEU:HD13	1:B:381:ARG:CZ	2.47	0.44
1:A:58:LYS:O	1:A:62:ILE:HG13	2.18	0.44
1:A:587:ASP:CG	1:A:588:ARG:H	2.21	0.44
1:B:249:SER:HB2	1:B:252:LYS:HE2	1.99	0.44
1:A:102:MET:HB3	1:A:107:ILE:HB	2.00	0.44
1:A:375:ARG:NH2	1:A:405:ARG:HB2	2.33	0.44
1:B:108:PHE:CD1	1:B:108:PHE:N	2.86	0.44
1:A:244:MET:HG3	1:A:247:MET:SD	2.58	0.44
1:A:120:GLN:HB3	1:A:205:TYR:CZ	2.53	0.44
1:B:435:HIS:O	1:B:437:LYS:HD2	2.17	0.44
1:B:264:TYR:HE1	1:B:288:ILE:HG22	1.83	0.43
1:B:398:VAL:HG12	1:B:400:VAL:CG1	2.48	0.43
1:B:296:ASN:OD1	1:B:298:LYS:HE2	2.18	0.43
1:A:249:SER:HB2	1:A:252:LYS:HE2	1.99	0.43
1:A:564:ARG:HG3	1:A:565:GLY:N	2.31	0.43
1:B:557:VAL:HA	1:B:558:PRO:HD3	1.89	0.43
1:B:244:MET:HG3	1:B:247:MET:SD	2.58	0.43
1:B:223:TYR:CZ	1:B:269:PRO:HD3	2.53	0.43
1:A:594:ARG:HB2	1:A:609:SER:O	2.18	0.43
1:A:373:ILE:HG23	1:A:376:VAL:CG1	2.47	0.43
1:B:150:LEU:HA	1:B:150:LEU:HD12	1.78	0.43
1:B:235:LEU:HD21	1:B:433:LYS:HZ1	1.83	0.43
1:B:235:LEU:HD21	1:B:433:LYS:NZ	2.33	0.43
1:B:120:GLN:HB3	1:B:205:TYR:CZ	2.53	0.43
1:B:611:ALA:HB2	1:B:623:GLU:HB3	2.00	0.43
1:B:12:LEU:HD11	1:B:79:LYS:HD2	2.00	0.43
1:B:83:ARG:HG2	1:B:83:ARG:NH1	2.32	0.43
1:A:569:LEU:C	1:A:569:LEU:HD23	2.38	0.43
1:B:628:LEU:HA	4:B:722:HOH:O	2.19	0.43
1:B:477:ASP:OD1	1:B:479:ARG:HD3	2.18	0.43
1:B:615:THR:HG22	1:B:620:TYR:HE1	1.83	0.43
1:B:520:ARG:NH1	1:B:605:LYS:HZ3	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ARG:CZ	1:A:590:LEU:HD21	2.48	0.43
1:B:46:LEU:O	1:B:49:PHE:HB3	2.18	0.43
1:B:266:ARG:HG2	1:B:266:ARG:HH11	1.84	0.43
1:A:534:THR:HB	1:A:597:ILE:HB	2.00	0.43
1:B:123:LEU:HA	1:B:123:LEU:HD23	1.91	0.43
1:B:375:ARG:NH2	1:B:405:ARG:HB2	2.34	0.43
1:A:146:LEU:O	1:A:147:VAL:C	2.57	0.43
1:B:542:ASP:O	1:B:546:VAL:HG23	2.19	0.43
1:A:108:PHE:CD1	1:A:108:PHE:N	2.86	0.43
1:B:345:TYR:HB3	1:B:346:PRO:HA	2.01	0.43
1:B:58:LYS:O	1:B:62:ILE:HG13	2.19	0.43
1:A:520:ARG:HH11	1:A:605:LYS:HZ3	1.66	0.43
1:B:372:ASN:HD22	1:B:438:LEU:H	1.67	0.43
1:B:659:SER:OG	1:B:661:ARG:HG3	2.19	0.42
1:B:233:TYR:CE1	1:B:236:VAL:HB	2.54	0.42
1:A:223:TYR:CZ	1:A:269:PRO:HD3	2.54	0.42
1:B:131:LEU:O	1:B:132:ARG:C	2.58	0.42
1:B:349:THR:CG2	1:B:351:GLU:HB2	2.50	0.42
1:A:345:TYR:HB3	1:A:346:PRO:HA	2.00	0.42
1:A:372:ASN:HD22	1:A:438:LEU:H	1.67	0.42
1:A:312:VAL:HG21	4:A:734:HOH:O	2.19	0.42
1:A:233:TYR:CE1	1:A:236:VAL:HB	2.54	0.42
1:A:179:VAL:CG1	1:A:180:PRO:HD2	2.42	0.42
1:B:618:ILE:HD12	1:B:618:ILE:N	2.34	0.42
1:B:594:ARG:CD	1:B:612:ASP:OD1	2.63	0.42
1:A:354:LEU:HD13	1:A:381:ARG:CZ	2.50	0.42
1:A:477:ASP:OD1	1:A:479:ARG:HD3	2.19	0.42
1:A:296:ASN:OD1	1:A:298:LYS:HE2	2.19	0.42
1:B:318:ARG:CZ	1:B:466:ARG:HG2	2.50	0.42
1:A:398:VAL:HG12	1:A:400:VAL:CG1	2.48	0.42
1:A:87:ALA:HA	1:A:90:GLU:OE1	2.19	0.42
1:B:87:ALA:HA	1:B:90:GLU:OE1	2.20	0.42
1:B:225:MET:HE1	1:B:276:LEU:HD22	2.02	0.42
1:A:77:LEU:CD2	1:A:77:LEU:H	2.32	0.41
1:B:77:LEU:CD2	1:B:77:LEU:H	2.33	0.41
1:B:323:TRP:CZ2	1:B:329:PHE:HZ	2.38	0.41
1:A:63:ILE:HA	1:A:251:LEU:HD21	2.02	0.41
1:A:611:ALA:HB2	1:A:623:GLU:HB3	2.02	0.41
1:B:648:THR:HB	1:B:665:ARG:HB3	2.01	0.41
1:B:261:ARG:HB3	1:B:261:ARG:HE	1.75	0.41
1:B:158:ALA:HA	1:B:171:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:TYR:HE1	1:A:288:ILE:HG22	1.84	0.41
1:B:79:LYS:O	1:B:83:ARG:HD2	2.18	0.41
1:A:451:ARG:HB2	1:A:481:THR:HG23	2.02	0.41
1:A:498:VAL:CG1	1:A:499:THR:N	2.83	0.41
1:A:233:TYR:CD1	1:A:236:VAL:HB	2.55	0.41
1:B:379:ASP:HA	1:B:414:TRP:HH2	1.83	0.41
1:A:464:THR:C	1:A:466:ARG:H	2.24	0.41
1:B:451:ARG:HB2	1:B:481:THR:HG23	2.01	0.41
1:B:264:TYR:CE1	1:B:288:ILE:HG22	2.55	0.41
1:A:235:LEU:HD21	1:A:433:LYS:HZ1	1.86	0.41
1:B:402:LEU:HD23	1:B:403:GLN:HG3	2.01	0.41
1:B:564:ARG:NE	1:B:590:LEU:HD21	2.35	0.41
1:B:536:LYS:O	1:B:594:ARG:HA	2.21	0.41
1:A:648:THR:HB	1:A:665:ARG:HB3	2.03	0.41
1:B:398:VAL:HG12	1:B:400:VAL:HG13	2.03	0.41
1:B:125:HIS:CE1	1:B:129:GLN:HG3	2.56	0.41
1:B:534:THR:HB	1:B:597:ILE:HB	2.02	0.41
1:A:46:LEU:O	1:A:49:PHE:HB3	2.21	0.41
1:A:190:PRO:HG2	1:A:193:ARG:HD3	2.03	0.41
1:B:590:LEU:HD11	3:B:704:ATP:H5'2	2.02	0.41
1:A:326:LYS:HE2	1:A:688:GLU:OE2	2.20	0.41
1:A:251:LEU:HD23	1:A:255:LEU:HG	2.03	0.40
1:B:233:TYR:CD1	1:B:236:VAL:HB	2.55	0.40
1:A:437:LYS:HE3	1:A:459:ASN:CA	2.51	0.40
1:A:401:GLU:C	1:A:403:GLN:H	2.24	0.40
1:A:546:VAL:HG12	1:A:550:TYR:CE1	2.56	0.40
1:A:322:ILE:HD13	1:A:322:ILE:HA	1.80	0.40
1:B:146:LEU:O	1:B:147:VAL:C	2.59	0.40
1:B:616:ARG:HA	1:B:620:TYR:HD1	1.86	0.40
1:A:264:TYR:CE1	1:A:288:ILE:HG22	2.56	0.40
1:A:402:LEU:HD23	1:A:403:GLN:HG3	2.03	0.40
1:A:131:LEU:HD21	1:A:179:VAL:HG11	2.03	0.40
1:A:223:TYR:HE2	1:A:267:ASP:HB2	1.87	0.40
1:B:272:LEU:HD22	1:B:276:LEU:HD11	2.03	0.40
1:B:66:GLU:HG2	1:B:254:ARG:HH11	1.86	0.40
1:B:435:HIS:HE1	1:B:594:ARG:HH22	1.69	0.40
1:A:83:ARG:HG2	1:A:83:ARG:NH1	2.35	0.40
1:A:375:ARG:HH22	1:A:405:ARG:HD2	1.87	0.40
1:A:9:GLU:HG2	1:A:9:GLU:H	1.68	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	685/687 (100%)	623 (91%)	47 (7%)	15 (2%)	8	13
1	B	685/687 (100%)	626 (91%)	44 (6%)	15 (2%)	8	13
All	All	1370/1374 (100%)	1249 (91%)	91 (7%)	30 (2%)	8	13

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	ALA
1	A	430	PRO
1	A	510	SER
1	B	189	ALA
1	B	430	PRO
1	B	510	SER
1	A	117	VAL
1	A	147	VAL
1	A	148	GLN
1	B	117	VAL
1	B	147	VAL
1	B	148	GLN
1	A	5	LYS
1	A	149	PHE
1	A	233	TYR
1	A	283	SER
1	A	414	TRP
1	A	666	GLY
1	B	5	LYS
1	B	149	PHE
1	B	233	TYR
1	B	283	SER
1	B	414	TRP
1	B	666	GLY
1	A	404	ALA

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Mol	Chain	Res	Type
1	A	687	PRO
1	B	404	ALA
1	B	687	PRO
1	A	673	ALA
1	B	673	ALA

### 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	619/619 (100%)	573 (93%)	46 (7%)	17	31
1	B	619/619 (100%)	574 (93%)	45 (7%)	17	32
All	All	1238/1238 (100%)	1147 (93%)	91 (7%)	17	31

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	64	SER
1	A	66	GLU
1	A	83	ARG
1	A	143	ASP
1	A	147	VAL
1	A	153	ASP
1	A	177	ASP
1	A	196	MET
1	A	230	ASP
1	A	234	ASP
1	A	244	MET
1	A	251	LEU
1	A	253	GLN
1	A	267	ASP
1	A	272	LEU
1	A	285	TYR
1	A	314	LYS

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Mol	Chain	Res	Type
1	A	343	LEU
1	A	349	THR
1	A	356	LEU
1	A	384	ASP
1	A	406	PHE
1	A	414	TRP
1	A	417	ARG
1	A	424	HIS
1	A	430	PRO
1	A	434	ILE
1	A	437	LYS
1	A	439	PHE
1	A	464	THR
1	A	468	TYR
1	A	472	SER
1	A	474	LEU
1	A	481	THR
1	A	496	ARG
1	A	548	ARG
1	A	564	ARG
1	A	590	LEU
1	A	596	TYR
1	A	616	ARG
1	A	626	THR
1	A	656	LYS
1	A	657	GLU
1	A	668	ARG
1	A	687	PRO
1	B	22	LEU
1	B	64	SER
1	B	66	GLU
1	B	83	ARG
1	B	143	ASP
1	B	147	VAL
1	B	153	ASP
1	B	177	ASP
1	B	196	MET
1	B	230	ASP
1	B	234	ASP
1	B	244	MET
1	B	251	LEU
1	B	253	GLN

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Mol	Chain	Res	Type
1	B	267	ASP
1	B	272	LEU
1	B	285	TYR
1	B	314	LYS
1	B	343	LEU
1	B	349	THR
1	B	356	LEU
1	B	384	ASP
1	B	406	PHE
1	B	414	TRP
1	B	417	ARG
1	B	424	HIS
1	B	430	PRO
1	B	434	ILE
1	B	437	LYS
1	B	439	PHE
1	B	464	THR
1	B	468	TYR
1	B	472	SER
1	B	474	LEU
1	B	481	THR
1	B	496	ARG
1	B	548	ARG
1	B	564	ARG
1	B	590	LEU
1	B	616	ARG
1	B	626	THR
1	B	656	LYS
1	B	657	GLU
1	B	668	ARG
1	B	687	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	114	GLN
1	A	121	ASN
1	A	253	GLN
1	A	265	GLN
1	A	270	ASN
1	A	348	HIS

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Mol	Chain	Res	Type
1	A	391	HIS
1	A	403	GLN
1	A	446	ASN
1	A	509	ASN
1	A	527	GLN
1	A	539	ASN
1	A	617	ASN
1	B	75	HIS
1	B	114	GLN
1	B	121	ASN
1	B	253	GLN
1	B	265	GLN
1	B	313	ASN
1	B	348	HIS
1	B	403	GLN
1	B	446	ASN
1	B	509	ASN
1	B	527	GLN
1	B	539	ASN
1	B	617	ASN

### 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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	701	2	24,33,33	3.08	10 (41%)	31,52,52	3.84	14 (45%)
3	ATP	B	704	2	24,33,33	2.62	7 (29%)	31,52,52	3.49	12 (38%)

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	701	2	-	0/18/38/38	0/3/3/3
3	ATP	B	704	2	-	0/18/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	ATP	O5'-C5'	-6.45	1.18	1.44
3	A	701	ATP	C3'-C4'	-4.16	1.41	1.53
3	B	704	ATP	O5'-C5'	-3.12	1.32	1.44
3	B	704	ATP	O2'-C2'	-2.17	1.37	1.43
3	B	704	ATP	C5'-C4'	-2.02	1.45	1.51
3	A	701	ATP	PG-O1G	2.14	1.58	1.51
3	A	701	ATP	O3'-C3'	2.17	1.48	1.43
3	B	704	ATP	C2-N3	2.50	1.36	1.32
3	A	701	ATP	C2'-C3'	2.54	1.60	1.53
3	A	701	ATP	PA-O2A	2.57	1.65	1.54
3	B	704	ATP	O4'-C4'	2.67	1.51	1.45
3	A	701	ATP	O4'-C4'	2.84	1.51	1.45
3	A	701	ATP	C2-N3	3.76	1.38	1.32
3	B	704	ATP	C4-N3	6.11	1.44	1.35
3	A	701	ATP	O4'-C1'	6.25	1.49	1.41
3	A	701	ATP	C4-N3	8.67	1.48	1.35
3	B	704	ATP	O4'-C1'	8.84	1.52	1.41

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	704	ATP	O5'-PA-O1A	-6.98	82.53	109.62
3	A	701	ATP	O5'-PA-O1A	-6.97	82.56	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	704	ATP	O3A-PA-O5'	-5.76	87.65	102.94
3	A	701	ATP	C5'-C4'-C3'	-5.67	92.70	115.21
3	A	701	ATP	O3A-PA-O5'	-5.47	88.42	102.94
3	A	701	ATP	C4'-O4'-C1'	-5.25	103.95	109.72
3	B	704	ATP	C5'-C4'-C3'	-5.19	94.59	115.21
3	B	704	ATP	C4'-O4'-C1'	-3.01	106.41	109.72
3	A	701	ATP	O2B-PB-O3A	-2.37	94.35	105.09
3	B	704	ATP	N3-C2-N1	-2.07	127.31	128.89
3	B	704	ATP	O2A-PA-O1A	2.12	124.02	112.53
3	A	701	ATP	O2G-PG-O1G	2.12	117.42	110.58
3	A	701	ATP	O3'-C3'-C2'	2.21	119.01	111.83
3	A	701	ATP	O2A-PA-O1A	2.24	124.65	112.53
3	A	701	ATP	O4'-C1'-N9	2.43	113.19	108.10
3	A	701	ATP	C4-C5-N7	2.67	111.93	109.48
3	B	704	ATP	O2A-PA-O3A	2.69	117.31	105.09
3	B	704	ATP	O2G-PG-O1G	2.70	119.27	110.58
3	A	701	ATP	O2B-PB-O3B	2.76	117.62	105.09
3	B	704	ATP	O2B-PB-O3B	2.99	118.68	105.09
3	A	701	ATP	O4'-C4'-C5'	3.00	120.04	109.32
3	B	704	ATP	O3'-C3'-C4'	3.17	120.57	111.05
3	B	704	ATP	C4-C5-N7	3.60	112.79	109.48
3	A	701	ATP	O4'-C4'-C3'	6.63	118.51	105.15
3	B	704	ATP	O5'-C5'-C4'	13.23	157.90	109.12
3	A	701	ATP	O5'-C5'-C4'	14.09	161.08	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	ATP	2	0
3	B	704	ATP	6	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	687/687 (100%)	0.56	81 (11%) 6 6	9, 29, 91, 136	0
1	B	687/687 (100%)	0.67	84 (12%) 5 5	8, 32, 92, 135	0
All	All	1374/1374 (100%)	0.62	165 (12%) 6 6	8, 30, 92, 136	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	405	ARG	13.7
1	A	239	MET	13.5
1	B	411	ASN	12.2
1	A	241	ALA	10.9
1	A	407	ASP	10.8
1	B	404	ALA	10.4
1	A	2	GLY	9.0
1	B	70	ASN	8.5
1	A	406	PHE	8.1
1	A	412	ILE	7.9
1	A	240	GLU	7.9
1	B	413	HIS	7.8
1	A	404	ALA	7.8
1	B	407	ASP	7.7
1	B	405	ARG	7.7
1	B	2	GLY	7.6
1	B	410	ALA	7.6
1	B	239	MET	7.6
1	A	70	ASN	7.6
1	A	411	ASN	7.4
1	B	406	PHE	7.3
1	A	238	GLU	7.3
1	B	243	LEU	7.3
1	B	408	GLU	7.2

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Mol	Chain	Res	Type	RSRZ
1	B	412	ILE	7.2
1	B	3	GLN	7.1
1	A	242	SER	7.0
1	B	414	TRP	6.7
1	B	188	GLU	6.5
1	A	235	LEU	6.4
1	A	408	GLU	6.3
1	B	240	GLU	6.2
1	B	403	GLN	6.1
1	B	192	ARG	5.8
1	B	4	GLU	5.8
1	B	71	SER	5.7
1	B	378	LYS	5.6
1	B	688	GLU	5.6
1	A	3	GLN	5.6
1	A	409	GLU	5.5
1	B	69	SER	5.4
1	A	285	TYR	5.2
1	B	191	ARG	5.2
1	A	414	TRP	5.2
1	B	246	LEU	5.0
1	A	688	GLU	5.0
1	B	235	LEU	4.8
1	A	429	ALA	4.8
1	A	237	HIS	4.8
1	A	191	ARG	4.8
1	A	244	MET	4.8
1	B	285	TYR	4.7
1	A	257	ALA	4.6
1	A	410	ALA	4.6
1	A	188	GLU	4.6
1	A	667	ASN	4.4
1	B	236	VAL	4.4
1	B	667	ASN	4.4
1	A	256	THR	4.3
1	B	237	HIS	4.2
1	A	413	HIS	4.2
1	B	234	ASP	4.2
1	A	374	TYR	4.2
1	A	4	GLU	4.2
1	B	374	TYR	4.2
1	A	236	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	409	GLU	4.1
1	A	415	ALA	4.1
1	B	241	ALA	4.0
1	A	243	LEU	4.0
1	B	574	GLU	4.0
1	A	117	VAL	3.9
1	A	148	GLN	3.9
1	B	377	ALA	3.8
1	B	620	TYR	3.8
1	A	378	LYS	3.8
1	A	234	ASP	3.8
1	B	244	MET	3.7
1	A	403	GLN	3.7
1	B	402	LEU	3.6
1	A	253	GLN	3.6
1	B	669	ARG	3.6
1	B	189	ALA	3.6
1	B	256	THR	3.5
1	B	249	SER	3.5
1	B	72	HIS	3.5
1	B	429	ALA	3.4
1	B	257	ALA	3.4
1	A	254	ARG	3.4
1	B	232	GLU	3.3
1	A	375	ARG	3.2
1	A	71	SER	3.2
1	A	661	ARG	3.2
1	B	194	LYS	3.2
1	B	253	GLN	3.2
1	A	258	GLU	3.2
1	B	415	ALA	3.2
1	A	314	LYS	3.1
1	A	143	ASP	3.1
1	A	245	GLU	3.1
1	B	575	GLY	3.1
1	B	314	LYS	3.0
1	A	192	ARG	3.0
1	B	190	PRO	3.0
1	B	148	GLN	3.0
1	A	189	ALA	3.0
1	A	669	ARG	3.0
1	B	247	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	291	GLY	2.9
1	B	238	GLU	2.9
1	B	686	GLN	2.8
1	A	402	LEU	2.8
1	B	193	ARG	2.8
1	B	661	ARG	2.8
1	B	5	LYS	2.7
1	B	233	TYR	2.7
1	B	68	GLY	2.7
1	B	665	ARG	2.7
1	A	284	ARG	2.7
1	B	251	LEU	2.6
1	B	430	PRO	2.6
1	A	232	GLU	2.6
1	A	74	ARG	2.6
1	A	252	LYS	2.6
1	A	376	VAL	2.5
1	B	266	ARG	2.5
1	A	129	GLN	2.5
1	B	254	ARG	2.5
1	B	417	ARG	2.5
1	A	428	SER	2.5
1	B	287	SER	2.5
1	B	432	LEU	2.5
1	A	377	ALA	2.5
1	A	246	LEU	2.4
1	B	520	ARG	2.4
1	A	280	LEU	2.4
1	B	245	GLU	2.4
1	A	247	MET	2.4
1	A	666	GLY	2.4
1	A	65	GLU	2.4
1	A	251	LEU	2.3
1	B	373	ILE	2.3
1	B	142	PRO	2.3
1	B	376	VAL	2.3
1	A	430	PRO	2.2
1	A	73	SER	2.2
1	A	282	ILE	2.2
1	A	574	GLU	2.2
1	A	72	HIS	2.2
1	B	666	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	466	ARG	2.2
1	A	158	ALA	2.2
1	A	124	ARG	2.1
1	A	310	ASN	2.1
1	B	306	VAL	2.1
1	B	307	GLY	2.1
1	A	177	ASP	2.1
1	B	261	ARG	2.1
1	B	446	ASN	2.1
1	B	145	ASP	2.1
1	A	248	SER	2.1
1	A	193	ARG	2.0
1	A	417	ARG	2.0
1	B	284	ARG	2.0
1	A	427	PHE	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	B	704	31/31	0.74	0.64	3.57	61,65,67,68	0
3	ATP	A	701	31/31	0.46	0.69	2.14	59,67,71,71	0
2	MG	B	705	1/1	0.80	1.19	-	68,68,68,68	0
2	MG	A	703	1/1	0.52	1.08	-	79,79,79,79	0
2	MG	A	702	1/1	0.57	0.57	-	58,58,58,58	0
2	MG	B	706	1/1	0.90	0.69	-	88,88,88,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.