



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2017 – 03:45 PM EDT

PDB ID : 3KX2  
Title : Crystal structure of Prp43p in complex with ADP  
Authors : Nielsen, K.H.; Andersen, G.R.; He, Y.  
Deposited on : unknown  
Resolution : 2.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

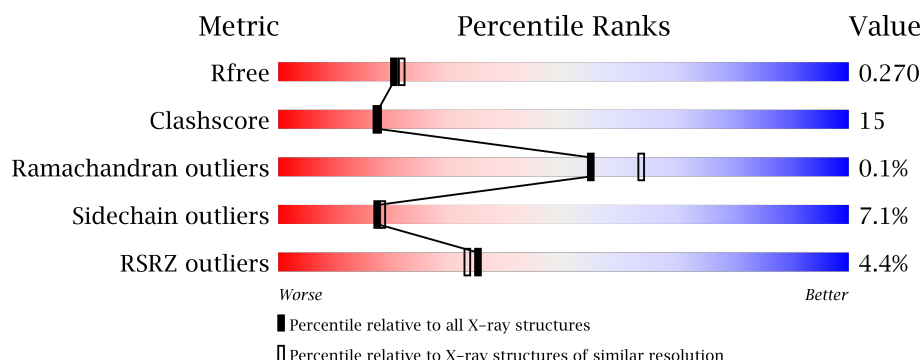
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	767	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>
1	B	767	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>5% •</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13172 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.

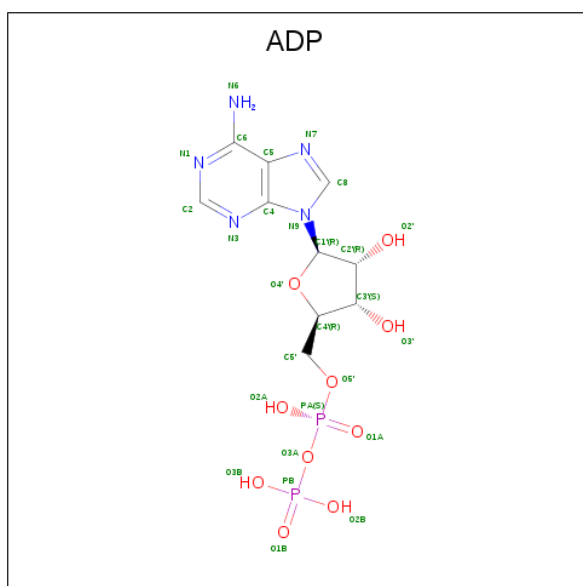
- Molecule 1 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP43.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	755	Total	C	N	O	S	0	0	0
			6067	3841	1048	1153	25			
1	A	755	Total	C	N	O	S	0	0	0
			6067	3841	1048	1153	25			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

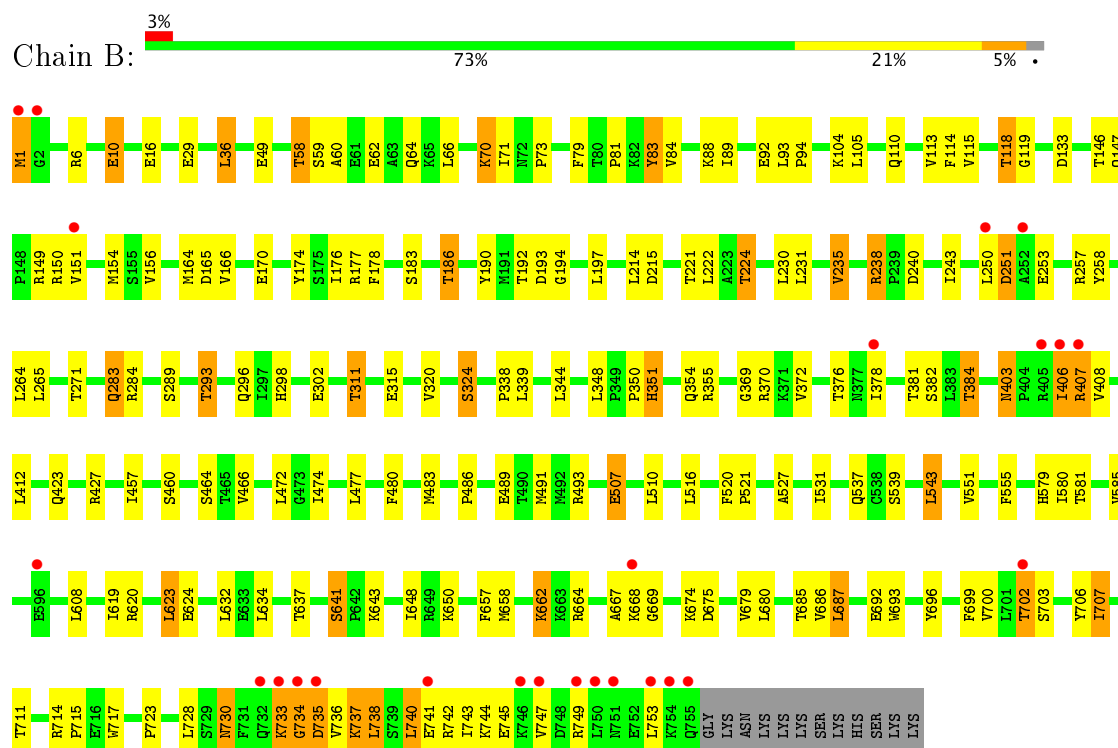
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	538	Total	O	0	0
			538	538		
4	A	444	Total	O	0	0
			444	444		

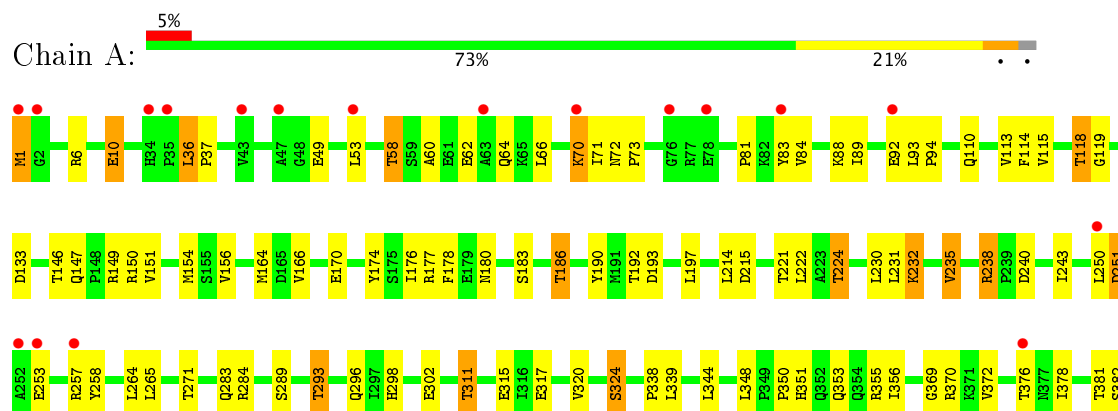
### 3 Residue-property plots [i](#)

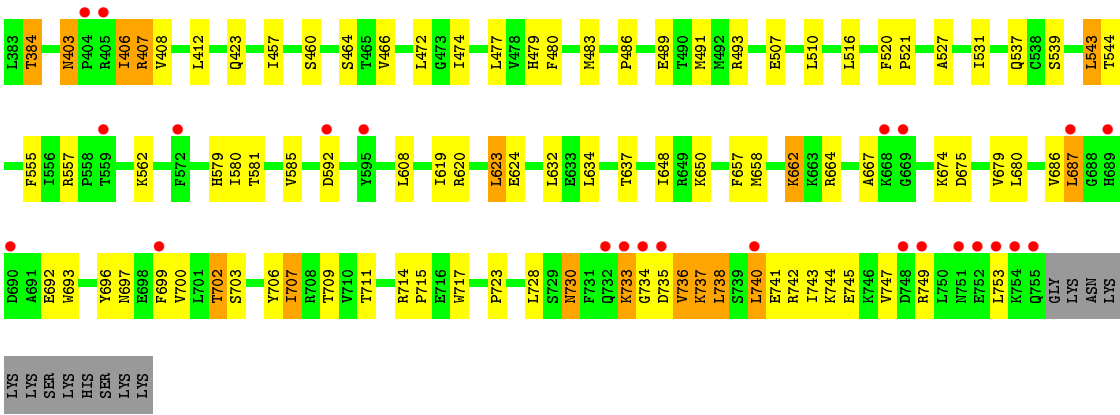
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP43



- Molecule 1: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP43





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.15Å 118.15Å 253.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.42 – 2.20 48.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.42-2.20) 99.8 (48.42-2.20)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.60 (at 2.20Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.206 , 0.250 0.238 , 0.270	Depositor DCC
$R_{free}$ test set	5220 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13172	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: MG, 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	0.71	18/6195 (0.3%)	0.58	6/8384 (0.1%)
1	B	0.59	16/6195 (0.3%)	0.61	9/8384 (0.1%)
All	All	0.65	34/12390 (0.3%)	0.59	15/16768 (0.1%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	317	GLU	CD-OE2	-17.97	1.05	1.25
1	A	317	GLU	CD-OE1	-17.68	1.06	1.25
1	A	83	TYR	CE2-CZ	-17.41	1.16	1.38
1	B	83	TYR	CD1-CE1	-17.22	1.13	1.39
1	B	83	TYR	CD2-CE2	-15.92	1.15	1.39
1	A	83	TYR	CD2-CE2	-13.93	1.18	1.39
1	B	215	ASP	C-O	-13.37	0.97	1.23
1	A	544	THR	C-O	-12.34	0.99	1.23
1	A	83	TYR	CG-CD1	-11.01	1.24	1.39
1	A	83	TYR	CD1-CE1	-10.31	1.23	1.39
1	A	317	GLU	CG-CD	-10.04	1.36	1.51
1	A	317	GLU	CB-CG	-9.70	1.33	1.52
1	B	83	TYR	CE1-CZ	-9.05	1.26	1.38
1	A	317	GLU	C-O	-9.04	1.06	1.23
1	A	215	ASP	CG-OD2	-8.93	1.04	1.25
1	A	544	THR	CB-CG2	-8.74	1.23	1.52
1	B	271	THR	C-O	-8.50	1.07	1.23
1	A	215	ASP	C-O	-8.50	1.07	1.23
1	A	83	TYR	CZ-OH	-8.37	1.23	1.37
1	B	83	TYR	CZ-OH	-8.14	1.24	1.37
1	B	83	TYR	C-O	-8.13	1.07	1.23
1	B	83	TYR	CE2-CZ	-8.06	1.28	1.38
1	A	215	ASP	CG-OD1	-7.66	1.07	1.25
1	B	215	ASP	CG-OD2	-7.37	1.08	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	83	TYR	CG-CD1	-6.96	1.30	1.39
1	B	271	THR	CA-C	-6.05	1.37	1.52
1	B	685	THR	C-O	-6.03	1.11	1.23
1	B	215	ASP	CG-OD1	-5.96	1.11	1.25
1	B	685	THR	CB-CG2	-5.63	1.33	1.52
1	B	685	THR	CB-OG1	-5.61	1.32	1.43
1	A	271	THR	C-O	-5.43	1.13	1.23
1	A	544	THR	CA-C	-5.35	1.39	1.52
1	B	271	THR	CB-OG1	-5.18	1.32	1.43
1	A	83	TYR	CE1-CZ	-5.10	1.31	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	734	GLY	N-CA-C	12.59	144.58	113.10
1	B	215	ASP	CB-CG-OD1	9.86	127.17	118.30
1	A	232	LYS	CB-CA-C	9.33	129.06	110.40
1	B	733	LYS	N-CA-C	8.59	134.18	111.00
1	A	215	ASP	CB-CG-OD1	8.56	126.01	118.30
1	A	733	LYS	N-CA-C	8.45	133.82	111.00
1	B	351	HIS	CB-CA-C	7.79	125.98	110.40
1	B	733	LYS	CB-CA-C	-7.57	95.27	110.40
1	A	733	LYS	CB-CA-C	-7.32	95.77	110.40
1	A	734	GLY	N-CA-C	7.20	131.11	113.10
1	A	317	GLU	OE1-CD-OE2	-7.02	114.87	123.30
1	B	685	THR	CB-CA-C	-6.27	94.68	111.60
1	B	641	SER	CB-CA-C	-6.18	98.36	110.10
1	B	215	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	B	271	THR	CA-CB-CG2	5.71	120.39	112.40

There are no chirality outliers.

There are no planarity outliers.

## 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	6067	0	6035	184	0
1	B	6067	0	6035	185	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	2	0
3	B	27	0	12	3	0
4	A	444	0	0	14	0
4	B	538	0	0	19	0
All	All	13172	0	12094	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 15.

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:A:70:LYS:HE2	1:A:70:LYS:H	1.13	1.13
1:B:735:ASP:HB2	1:B:737:LYS:HE3	1.27	1.13
1:B:70:LYS:HE2	1:B:70:LYS:H	1.13	1.13
1:A:737:LYS:H	1:A:737:LYS:HE2	1.10	1.12
1:B:737:LYS:H	1:B:737:LYS:HE2	1.10	1.11
1:B:407:ARG:HH11	1:B:407:ARG:HG3	1.17	1.05
1:A:407:ARG:HG3	1:A:407:ARG:HH11	1.18	1.05
1:B:693:TRP:CD1	1:B:715:PRO:HG3	1.97	0.99
1:A:693:TRP:CD1	1:A:715:PRO:HG3	1.98	0.99
1:A:737:LYS:HD2	1:A:738:LEU:H	1.26	0.97
1:B:679:VAL:HG21	1:B:707:ILE:HD12	1.45	0.96
1:A:679:VAL:HG21	1:A:707:ILE:HD12	1.48	0.95
1:B:737:LYS:HD2	1:B:738:LEU:H	1.28	0.94
1:A:146:THR:HG22	1:A:214:LEU:HA	1.55	0.86
1:B:146:THR:HG22	1:B:214:LEU:HA	1.56	0.86
1:B:700:VAL:HG13	1:B:706:TYR:HB2	1.57	0.85
1:A:700:VAL:HG13	1:A:706:TYR:HB2	1.57	0.85
1:B:728:LEU:HD12	1:B:728:LEU:H	1.43	0.84
1:A:115:VAL:HG11	1:A:250:LEU:HA	1.60	0.83
1:B:115:VAL:HG11	1:B:250:LEU:HA	1.60	0.83
1:B:735:ASP:HB2	1:B:737:LYS:CE	2.09	0.83
1:B:6:ARG:HB3	4:B:957:HOH:O	1.78	0.82
1:B:70:LYS:HE2	1:B:70:LYS:N	1.96	0.81
1:A:728:LEU:HD12	1:A:728:LEU:H	1.46	0.80
1:B:407:ARG:HH11	1:B:407:ARG:CG	1.94	0.80
1:A:737:LYS:HE2	1:A:737:LYS:N	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ARG:CG	1:A:407:ARG:HH11	1.95	0.79
1:B:555:PHE:CZ	1:B:585:VAL:HG21	2.17	0.78
1:A:183:SER:H	1:A:186:THR:HG23	1.47	0.78
1:B:737:LYS:N	1:B:737:LYS:HE2	1.94	0.78
1:B:183:SER:H	1:B:186:THR:HG23	1.50	0.77
1:B:311:THR:HB	1:B:315:GLU:OE1	1.86	0.75
1:A:555:PHE:CZ	1:A:585:VAL:HG21	2.21	0.75
1:B:555:PHE:HZ	1:B:585:VAL:HG21	1.53	0.74
1:A:311:THR:HB	1:A:315:GLU:OE1	1.86	0.74
1:B:687:LEU:H	1:B:687:LEU:HD23	1.53	0.74
1:A:183:SER:H	1:A:186:THR:CG2	2.00	0.73
1:A:70:LYS:N	1:A:70:LYS:HE2	1.96	0.72
1:B:70:LYS:CE	1:B:70:LYS:H	1.98	0.72
1:A:687:LEU:H	1:A:687:LEU:HD23	1.53	0.71
1:A:70:LYS:CE	1:A:70:LYS:H	1.99	0.71
1:A:735:ASP:HB2	1:A:737:LYS:HE3	1.71	0.71
3:B:1000:ADP:H5'1	3:B:1000:ADP:N3	2.06	0.71
1:B:183:SER:H	1:B:186:THR:CG2	2.03	0.71
1:A:736:VAL:H	1:A:737:LYS:HE2	1.56	0.70
1:A:376:THR:HG23	1:A:378:ILE:H	1.55	0.70
1:A:146:THR:OG1	1:A:193:ASP:HA	1.92	0.70
1:B:146:THR:OG1	1:B:193:ASP:HA	1.93	0.69
1:B:376:THR:HG23	1:B:378:ILE:H	1.57	0.69
1:A:737:LYS:CD	1:A:738:LEU:H	2.03	0.69
1:A:555:PHE:HZ	1:A:585:VAL:HG21	1.58	0.69
1:A:477:LEU:HB3	1:A:491:MET:CE	2.23	0.68
1:B:477:LEU:HB3	1:B:491:MET:CE	2.23	0.67
1:B:253:GLU:O	1:B:257:ARG:HG2	1.94	0.67
1:A:737:LYS:CE	1:A:737:LYS:H	2.00	0.67
1:A:407:ARG:HG3	1:A:407:ARG:NH1	1.99	0.67
1:A:537:GLN:HB2	4:A:804:HOH:O	1.95	0.66
1:A:49:GLU:HG3	1:A:73:PRO:HA	1.78	0.66
1:A:693:TRP:CZ2	1:A:740:LEU:HD11	2.30	0.66
1:B:221:THR:OG1	1:B:224:THR:HG23	1.96	0.66
1:B:737:LYS:CD	1:B:738:LEU:H	2.05	0.66
1:B:118:THR:HG21	1:B:381:THR:HA	1.78	0.66
1:B:693:TRP:CZ2	1:B:740:LEU:HD11	2.31	0.66
1:A:221:THR:OG1	1:A:224:THR:HG23	1.96	0.65
1:A:58:THR:HB	1:A:133:ASP:OD2	1.97	0.65
1:B:477:LEU:HB3	1:B:491:MET:HE1	1.76	0.65
1:B:49:GLU:HG3	1:B:73:PRO:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1000:ADP:H5'1	3:A:1000:ADP:N3	2.11	0.65
1:B:736:VAL:H	1:B:737:LYS:HE2	1.60	0.65
1:B:114:PHE:CE2	1:B:265:LEU:HD22	2.32	0.65
1:A:298:HIS:HD2	1:A:370:ARG:HD2	1.62	0.65
1:A:702:THR:HG23	1:A:703:SER:H	1.62	0.65
1:B:384:THR:HG23	4:B:836:HOH:O	1.96	0.65
1:B:527:ALA:O	1:B:531:ILE:HG12	1.97	0.64
1:A:170:GLU:O	1:A:186:THR:HG22	1.98	0.64
1:B:702:THR:HG23	1:B:703:SER:H	1.61	0.64
1:B:737:LYS:H	1:B:737:LYS:CE	2.00	0.64
1:A:537:GLN:O	1:A:637:THR:HG23	1.98	0.64
1:B:298:HIS:HD2	1:B:370:ARG:HD2	1.61	0.64
1:A:479:HIS:HE1	4:A:937:HOH:O	1.80	0.63
1:A:253:GLU:O	1:A:257:ARG:HG2	1.97	0.63
1:A:662:LYS:HB3	1:A:662:LYS:NZ	2.13	0.63
1:B:715:PRO:HB2	1:B:744:LYS:HD3	1.81	0.63
1:B:58:THR:HB	1:B:133:ASP:OD2	1.99	0.63
1:A:737:LYS:HD2	1:A:738:LEU:N	2.08	0.62
1:A:298:HIS:CD2	1:A:370:ARG:HD2	2.35	0.62
3:B:1000:ADP:H2'	4:B:1167:HOH:O	2.00	0.61
1:B:662:LYS:NZ	1:B:662:LYS:HB3	2.15	0.61
1:B:170:GLU:O	1:B:186:THR:HG22	2.00	0.61
1:A:114:PHE:CE2	1:A:265:LEU:HD22	2.36	0.61
1:A:715:PRO:HB2	1:A:744:LYS:HD3	1.81	0.61
1:B:320:VAL:O	1:B:324:SER:HB2	2.00	0.61
1:A:527:ALA:O	1:A:531:ILE:HG12	2.01	0.60
1:B:298:HIS:CD2	1:B:370:ARG:HD2	2.36	0.60
1:A:118:THR:HG21	1:A:381:THR:HA	1.82	0.60
1:A:298:HIS:HD2	1:A:370:ARG:HH11	1.50	0.60
1:A:407:ARG:HD2	1:A:493:ARG:HH11	1.67	0.60
1:A:477:LEU:HB3	1:A:491:MET:HE3	1.84	0.60
1:B:537:GLN:O	1:B:637:THR:HG23	2.02	0.60
3:B:1000:ADP:C5'	3:B:1000:ADP:N3	2.65	0.60
1:B:104:LYS:HG2	4:B:893:HOH:O	2.02	0.59
1:B:118:THR:HG23	4:B:792:HOH:O	2.01	0.59
1:A:662:LYS:HG3	1:A:693:TRP:CZ2	2.38	0.59
1:A:113:VAL:HG23	1:A:264:LEU:HD12	1.85	0.59
1:B:744:LYS:HA	1:B:744:LYS:HE2	1.85	0.59
1:A:320:VAL:O	1:A:324:SER:HB2	2.02	0.58
1:B:298:HIS:HD2	1:B:370:ARG:HH11	1.50	0.58
1:B:407:ARG:HD2	1:B:493:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:LYS:HA	1:A:744:LYS:HE2	1.86	0.58
1:A:735:ASP:HB2	1:A:737:LYS:CE	2.33	0.58
1:B:384:THR:CG2	4:B:836:HOH:O	2.52	0.58
1:A:113:VAL:HG23	1:A:264:LEU:CD1	2.34	0.58
1:B:737:LYS:HD2	1:B:738:LEU:N	2.11	0.57
1:A:662:LYS:HE3	1:A:740:LEU:CD1	2.34	0.57
1:B:662:LYS:HG3	1:B:693:TRP:CZ2	2.39	0.57
1:A:679:VAL:HG21	1:A:707:ILE:CD1	2.27	0.57
1:B:193:ASP:OD2	1:B:224:THR:HG22	2.05	0.57
1:B:113:VAL:HG23	1:B:264:LEU:HD12	1.87	0.57
1:B:113:VAL:HG23	1:B:264:LEU:CD1	2.34	0.57
1:B:662:LYS:HE3	1:B:740:LEU:CD1	2.34	0.57
1:B:679:VAL:HG21	1:B:707:ILE:CD1	2.26	0.57
1:B:407:ARG:HG3	1:B:407:ARG:NH1	1.98	0.57
1:B:730:ASN:C	1:B:730:ASN:HD22	2.08	0.57
1:A:407:ARG:CG	1:A:407:ARG:NH1	2.61	0.57
1:A:592:ASP:HB3	4:A:1229:HOH:O	2.04	0.56
1:B:407:ARG:NH1	1:B:407:ARG:CG	2.60	0.56
1:A:1:MET:H1	1:A:1:MET:HE3	1.70	0.56
1:B:581:THR:O	1:B:585:VAL:HG23	2.06	0.56
1:A:53:LEU:HA	4:A:890:HOH:O	2.05	0.56
1:A:737:LYS:O	1:A:741:GLU:HG2	2.05	0.56
1:B:403:ASN:HB3	1:B:406:ILE:HG23	1.87	0.56
1:A:147:GLN:O	1:A:192:THR:HA	2.06	0.56
1:A:174:TYR:HA	1:A:190:TYR:O	2.05	0.56
1:B:737:LYS:O	1:B:741:GLU:HG2	2.05	0.56
1:B:79:PHE:CE1	1:B:83:TYR:CE2	2.94	0.56
1:A:477:LEU:HB3	1:A:491:MET:HE1	1.87	0.56
1:B:1:MET:H1	1:B:1:MET:HE3	1.71	0.56
1:A:581:THR:O	1:A:585:VAL:HG23	2.06	0.55
1:B:147:GLN:O	1:B:192:THR:HA	2.06	0.55
1:A:403:ASN:HB3	1:A:406:ILE:HG23	1.88	0.55
1:B:668:LYS:HG3	4:B:972:HOH:O	2.07	0.55
1:A:193:ASP:OD2	1:A:224:THR:HG22	2.07	0.54
1:B:83:TYR:CD2	1:B:165:ASP:HB2	2.42	0.54
1:A:730:ASN:HD22	1:A:730:ASN:C	2.09	0.54
1:B:289:SER:O	1:B:293:THR:HG22	2.06	0.54
1:A:423:GLN:HA	1:A:423:GLN:HE21	1.72	0.54
1:A:81:PRO:O	1:A:84:VAL:HG22	2.08	0.54
1:A:543:LEU:HD22	1:A:620:ARG:HG3	1.88	0.54
1:B:734:GLY:O	1:B:735:ASP:C	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:PRO:O	1:B:84:VAL:HG22	2.08	0.54
1:B:174:TYR:HA	1:B:190:TYR:O	2.08	0.53
1:B:289:SER:O	1:B:293:THR:CG2	2.56	0.53
1:B:339:LEU:HD11	1:B:372:VAL:CG2	2.38	0.53
3:A:1000:ADP:C5'	3:A:1000:ADP:N3	2.71	0.53
1:A:657:PHE:CE2	1:A:658:MET:HG3	2.43	0.53
1:B:376:THR:CG2	1:B:378:ILE:HG13	2.38	0.53
1:A:355:ARG:HD2	4:A:945:HOH:O	2.08	0.53
1:A:230:LEU:HD21	1:A:472:LEU:HD13	1.91	0.53
1:A:289:SER:O	1:A:293:THR:HG22	2.08	0.53
1:A:728:LEU:HB3	1:A:738:LEU:HD21	1.90	0.53
1:B:423:GLN:HE21	1:B:423:GLN:HA	1.73	0.53
1:B:728:LEU:HB3	1:B:738:LEU:HD21	1.91	0.53
1:A:662:LYS:HE2	1:A:736:VAL:CG1	2.39	0.53
1:B:662:LYS:HE2	1:B:736:VAL:CG1	2.39	0.53
1:A:119:GLY:HA2	1:A:384:THR:HG21	1.91	0.53
1:A:579:HIS:HE1	4:A:913:HOH:O	1.91	0.53
1:B:543:LEU:HD22	1:B:620:ARG:HG3	1.91	0.53
1:A:302:GLU:O	1:A:370:ARG:NH2	2.42	0.52
1:B:36:LEU:CD2	1:B:36:LEU:H	2.21	0.52
1:B:170:GLU:O	1:B:186:THR:HA	2.10	0.52
1:A:339:LEU:HD11	1:A:372:VAL:CG2	2.40	0.52
1:A:516:LEU:HD22	4:A:1070:HOH:O	2.09	0.52
1:B:406:ILE:HG13	1:B:406:ILE:O	2.10	0.52
4:B:1020:HOH:O	1:A:351:HIS:HD2	1.93	0.51
1:A:338:PRO:HD2	1:A:369:GLY:HA2	1.92	0.51
1:B:298:HIS:CD2	1:B:370:ARG:HH11	2.29	0.51
1:B:657:PHE:CE2	1:B:658:MET:HG3	2.46	0.51
1:A:406:ILE:HG13	1:A:406:ILE:O	2.11	0.51
1:A:619:ILE:HG22	1:A:623:LEU:HD22	1.93	0.51
1:A:693:TRP:HZ2	1:A:740:LEU:HD11	1.71	0.51
1:A:289:SER:O	1:A:293:THR:CG2	2.59	0.51
1:A:36:LEU:CD2	1:A:36:LEU:H	2.24	0.51
1:B:693:TRP:HZ2	1:B:740:LEU:HD11	1.73	0.51
1:B:149:ARG:HD2	1:B:382:SER:OG	2.11	0.50
1:A:531:ILE:HD13	1:A:632:LEU:HD11	1.92	0.50
1:A:150:ARG:NH2	1:A:348:LEU:O	2.44	0.50
1:B:539:SER:O	1:B:543:LEU:HB2	2.11	0.50
1:B:423:GLN:NE2	1:B:423:GLN:HA	2.27	0.50
1:B:619:ILE:HG22	1:B:623:LEU:HD22	1.94	0.50
1:A:231:LEU:O	1:A:232:LYS:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LYS:O	1:A:675:ASP:HB2	2.12	0.50
1:B:740:LEU:HD13	1:B:741:GLU:N	2.26	0.50
1:A:298:HIS:CD2	1:A:370:ARG:HH11	2.30	0.50
1:A:539:SER:O	1:A:543:LEU:HB2	2.12	0.50
1:A:692:GLU:HG3	1:A:693:TRP:HD1	1.77	0.50
1:B:119:GLY:HA2	1:B:384:THR:HG21	1.93	0.50
1:B:60:ALA:O	1:B:64:GLN:HG3	2.12	0.50
1:A:423:GLN:NE2	1:A:423:GLN:HA	2.26	0.50
1:A:180:ASN:HB2	4:A:1148:HOH:O	2.10	0.50
1:B:110:GLN:CD	1:B:235:VAL:HG22	2.32	0.50
1:B:738:LEU:HD13	1:B:742:ARG:NH2	2.27	0.50
1:B:302:GLU:HG2	4:B:1095:HOH:O	2.12	0.49
1:A:231:LEU:HB3	1:A:243:ILE:HD13	1.94	0.49
1:B:150:ARG:HG3	1:B:176:ILE:HG21	1.94	0.49
1:A:193:ASP:OD2	1:A:224:THR:CG2	2.60	0.49
1:A:6:ARG:HG2	4:A:1203:HOH:O	2.13	0.49
1:B:79:PHE:CE1	1:B:83:TYR:CZ	3.00	0.49
1:A:580:ILE:CD1	1:A:648:ILE:HG21	2.42	0.49
1:A:170:GLU:O	1:A:186:THR:HA	2.12	0.48
1:A:60:ALA:O	1:A:64:GLN:HG3	2.13	0.48
1:A:150:ARG:HG3	1:A:176:ILE:HG21	1.96	0.48
1:A:231:LEU:HB3	1:A:243:ILE:CD1	2.43	0.48
1:B:230:LEU:HD21	1:B:472:LEU:HD13	1.96	0.48
1:A:110:GLN:CD	1:A:235:VAL:HG22	2.34	0.48
1:A:230:LEU:HD11	1:A:472:LEU:HD13	1.96	0.48
1:B:477:LEU:HB3	1:B:491:MET:HE3	1.96	0.48
1:A:662:LYS:HG3	1:A:693:TRP:CE2	2.49	0.48
1:B:302:GLU:O	1:B:370:ARG:NH2	2.47	0.48
1:B:674:LYS:O	1:B:675:ASP:HB2	2.14	0.48
1:B:692:GLU:HG3	1:B:693:TRP:HD1	1.77	0.48
1:A:149:ARG:HD2	1:A:382:SER:OG	2.14	0.48
1:B:537:GLN:HG2	1:B:637:THR:HG22	1.96	0.48
1:A:740:LEU:HD13	1:A:741:GLU:N	2.28	0.48
1:B:183:SER:O	1:B:186:THR:HG23	2.14	0.47
1:B:407:ARG:HG2	1:B:407:ARG:O	2.14	0.47
1:A:466:VAL:HG13	1:A:477:LEU:HD11	1.97	0.47
1:A:714:ARG:HB2	1:A:717:TRP:CD2	2.50	0.47
1:B:193:ASP:OD2	1:B:224:THR:CG2	2.61	0.47
1:B:696:TYR:CB	1:B:707:ILE:HG23	2.44	0.47
1:A:738:LEU:HD13	1:A:742:ARG:NH2	2.30	0.47
1:B:1:MET:HA	4:B:1055:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:THR:CG2	1:A:214:LEU:HA	2.36	0.47
1:A:183:SER:O	1:A:186:THR:HG23	2.15	0.47
1:A:407:ARG:O	1:A:407:ARG:HG2	2.15	0.46
1:A:662:LYS:HB3	1:A:662:LYS:HZ3	1.80	0.46
1:A:696:TYR:CB	1:A:707:ILE:HG23	2.45	0.46
1:A:457:ILE:HD11	1:A:486:PRO:HG3	1.98	0.46
1:B:531:ILE:HD13	1:B:632:LEU:HD11	1.96	0.46
1:B:662:LYS:HG3	1:B:693:TRP:CE2	2.50	0.46
1:B:338:PRO:HD2	1:B:369:GLY:HA2	1.97	0.46
1:B:743:ILE:O	1:B:747:VAL:HG23	2.15	0.46
1:A:624:GLU:HG3	1:A:634:LEU:HD11	1.97	0.46
1:B:154:MET:CE	1:B:350:PRO:HG3	2.46	0.46
1:A:735:ASP:O	1:A:736:VAL:HG22	2.15	0.46
1:B:231:LEU:HB3	1:B:243:ILE:HD13	1.98	0.46
1:A:537:GLN:HG2	1:A:637:THR:HG22	1.97	0.46
1:B:466:VAL:HG13	1:B:477:LEU:HD11	1.98	0.46
1:B:579:HIS:HD2	1:B:711:THR:OG1	1.99	0.46
1:A:423:GLN:CA	1:A:423:GLN:HE21	2.28	0.46
1:B:230:LEU:HD11	1:B:472:LEU:HD13	1.97	0.46
1:A:736:VAL:O	1:A:740:LEU:HD12	2.16	0.45
1:A:693:TRP:CZ2	1:A:740:LEU:HD21	2.51	0.45
1:A:743:ILE:O	1:A:747:VAL:HG23	2.16	0.45
1:B:238:ARG:HB2	1:B:240:ASP:OD1	2.16	0.45
1:A:680:LEU:HD12	1:A:680:LEU:N	2.32	0.45
1:B:258:TYR:CG	1:B:483:MET:HE2	2.52	0.45
1:A:258:TYR:CG	1:A:483:MET:HE2	2.51	0.45
1:B:177:ARG:O	1:B:178:PHE:HB2	2.17	0.45
1:A:664:ARG:HD2	1:A:667:ALA:HB3	1.98	0.45
1:B:474:ILE:HD13	1:B:480:PHE:CE1	2.51	0.45
1:B:736:VAL:O	1:B:740:LEU:HD12	2.17	0.45
1:A:474:ILE:HD13	1:A:480:PHE:CE1	2.52	0.45
1:A:579:HIS:HD2	1:A:711:THR:OG1	2.00	0.45
1:B:624:GLU:HG3	1:B:634:LEU:HD11	1.99	0.45
1:B:680:LEU:HD12	1:B:680:LEU:N	2.32	0.45
1:B:714:ARG:HB2	1:B:717:TRP:CD2	2.52	0.45
1:B:693:TRP:CZ2	1:B:740:LEU:HD21	2.52	0.45
1:A:735:ASP:CB	1:A:737:LYS:HE3	2.43	0.45
1:B:146:THR:CG2	1:B:214:LEU:HA	2.39	0.44
1:B:579:HIS:HE1	4:B:994:HOH:O	2.00	0.44
1:A:177:ARG:O	1:A:178:PHE:HB2	2.17	0.44
1:A:376:THR:CG2	1:A:378:ILE:HG13	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:ASP:O	1:A:736:VAL:CG2	2.65	0.44
1:A:238:ARG:HB2	1:A:240:ASP:OD1	2.18	0.44
1:B:664:ARG:HD2	1:B:667:ALA:HB3	2.00	0.44
1:B:740:LEU:HD13	1:B:740:LEU:C	2.38	0.44
1:A:118:THR:HG23	4:A:942:HOH:O	2.16	0.44
1:A:214:LEU:HD11	1:A:231:LEU:HD12	2.00	0.44
1:A:740:LEU:HD23	4:A:918:HOH:O	2.18	0.44
1:A:10:GLU:HG2	1:A:10:GLU:H	1.46	0.44
1:B:16:GLU:HB2	4:B:816:HOH:O	2.18	0.44
1:B:231:LEU:HB3	1:B:243:ILE:CD1	2.47	0.44
1:B:150:ARG:NH2	1:B:348:LEU:O	2.51	0.44
1:B:723:PRO:HD2	4:B:1243:HOH:O	2.18	0.44
1:B:214:LEU:HD11	1:B:231:LEU:HD12	2.00	0.43
1:B:62:GLU:O	1:B:66:LEU:HD22	2.18	0.43
1:B:650:LYS:HE2	1:B:717:TRP:CD1	2.54	0.43
1:B:580:ILE:CD1	1:B:648:ILE:HG21	2.49	0.43
1:B:662:LYS:HB3	1:B:662:LYS:HZ3	1.82	0.43
1:B:543:LEU:HD13	1:B:620:ARG:CZ	2.48	0.43
1:A:115:VAL:CG1	1:A:250:LEU:HA	2.41	0.43
1:B:520:PHE:HA	1:B:521:PRO:HD3	1.91	0.43
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.85	0.43
1:B:10:GLU:HG2	1:B:10:GLU:H	1.46	0.43
1:B:350:PRO:O	1:B:351:HIS:C	2.54	0.43
1:B:354:GLN:NE2	4:B:1127:HOH:O	2.51	0.43
1:B:737:LYS:CG	1:B:738:LEU:N	2.82	0.43
1:B:58:THR:HG23	1:B:59:SER:N	2.34	0.43
1:A:403:ASN:O	1:A:407:ARG:N	2.51	0.43
1:A:740:LEU:HD13	1:A:740:LEU:C	2.39	0.43
1:A:744:LYS:CE	1:A:744:LYS:HA	2.49	0.42
1:B:745:GLU:O	1:B:749:ARG:HG3	2.19	0.42
1:B:151:VAL:HG11	1:B:344:LEU:HD11	2.00	0.42
1:B:403:ASN:O	1:B:407:ARG:N	2.51	0.42
1:A:737:LYS:CG	1:A:738:LEU:N	2.82	0.42
1:A:296:GLN:HE21	1:A:296:GLN:HB2	1.67	0.42
1:B:355:ARG:HD2	4:B:1146:HOH:O	2.19	0.42
1:B:88:LYS:HG3	1:B:89:ILE:N	2.34	0.42
1:B:296:GLN:HE21	1:B:296:GLN:HB2	1.67	0.42
1:B:93:LEU:HA	1:B:94:PRO:HD3	1.93	0.42
1:A:338:PRO:HD2	1:A:369:GLY:CA	2.49	0.42
1:A:479:HIS:CE1	4:A:937:HOH:O	2.63	0.42
1:B:302:GLU:HG2	1:B:302:GLU:H	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:PRO:HB2	1:B:744:LYS:CD	2.48	0.42
1:A:537:GLN:NE2	4:A:1128:HOH:O	2.52	0.42
1:A:93:LEU:HA	1:A:94:PRO:HD3	1.93	0.42
1:B:339:LEU:HD11	1:B:372:VAL:HG23	2.02	0.42
1:B:662:LYS:HE2	1:B:736:VAL:HG12	2.01	0.42
1:A:251:ASP:OD2	1:A:251:ASP:C	2.57	0.42
1:A:520:PHE:HA	1:A:521:PRO:HD3	1.93	0.42
1:A:723:PRO:HD2	4:A:912:HOH:O	2.20	0.42
1:B:744:LYS:CE	1:B:744:LYS:HA	2.49	0.42
1:A:733:LYS:N	1:A:733:LYS:HE2	2.35	0.41
1:A:88:LYS:HG3	1:A:89:ILE:N	2.35	0.41
1:B:164:MET:O	1:B:166:VAL:HG13	2.20	0.41
1:A:119:GLY:CA	1:A:384:THR:HG21	2.49	0.41
1:B:457:ILE:HD11	1:B:486:PRO:HG3	2.03	0.41
1:A:177:ARG:HG2	1:A:178:PHE:CD2	2.55	0.41
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.84	0.41
1:A:696:TYR:CD1	1:A:707:ILE:HD13	2.55	0.41
1:B:641:SER:O	1:B:643:LYS:N	2.53	0.41
1:A:353:GLN:O	1:A:356:ILE:HG12	2.21	0.41
1:A:697:ASN:HB3	1:A:709:THR:HB	2.02	0.41
1:B:516:LEU:CD2	1:B:531:ILE:HD12	2.51	0.41
1:B:733:LYS:HE2	1:B:733:LYS:N	2.36	0.41
1:B:734:GLY:HA2	4:B:1319:HOH:O	2.21	0.41
1:A:580:ILE:HD11	1:A:648:ILE:HG21	2.01	0.41
1:A:693:TRP:HZ2	1:A:740:LEU:HD21	1.85	0.41
1:A:745:GLU:O	1:A:749:ARG:HG3	2.19	0.41
1:B:283:GLN:HE21	1:B:283:GLN:CA	2.33	0.41
1:B:29:GLU:HB3	4:B:1190:HOH:O	2.20	0.41
1:B:507:GLU:HG3	4:B:1361:HOH:O	2.20	0.41
1:A:737:LYS:HZ3	1:A:737:LYS:HB3	1.86	0.41
1:B:88:LYS:HE2	1:B:88:LYS:HB2	1.90	0.41
1:A:62:GLU:O	1:A:66:LEU:HD22	2.21	0.41
1:B:664:ARG:HB2	1:B:669:GLY:O	2.20	0.41
1:B:423:GLN:CA	1:B:423:GLN:HE21	2.29	0.41
1:B:740:LEU:HD22	1:B:740:LEU:O	2.20	0.41
1:A:715:PRO:HB2	1:A:744:LYS:CD	2.48	0.41
1:A:154:MET:CE	1:A:350:PRO:HG3	2.51	0.41
1:B:251:ASP:C	1:B:251:ASP:OD2	2.59	0.41
1:B:36:LEU:N	1:B:36:LEU:HD23	2.36	0.41
1:A:164:MET:O	1:A:166:VAL:HG13	2.21	0.41
1:A:557:ARG:NH1	1:A:562:LYS:HD3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:LEU:HD12	1:A:623:LEU:HA	1.89	0.41
1:A:662:LYS:HE2	1:A:736:VAL:HG12	2.01	0.41
1:A:72:ASN:HA	1:A:73:PRO:HD3	1.97	0.41
1:B:696:TYR:CD1	1:B:707:ILE:HD13	2.56	0.41
1:A:151:VAL:HG11	1:A:344:LEU:HD11	2.03	0.40
1:A:537:GLN:CG	1:A:637:THR:HG22	2.52	0.40
1:B:194:GLY:HA3	4:B:838:HOH:O	2.20	0.40
1:B:36:LEU:H	1:B:36:LEU:HD23	1.87	0.40
1:B:537:GLN:CG	1:B:637:THR:HG22	2.51	0.40
1:A:176:ILE:HG22	1:A:177:ARG:N	2.37	0.40
1:A:650:LYS:HE2	1:A:717:TRP:CD1	2.57	0.40
1:B:177:ARG:HG2	1:B:178:PHE:CD2	2.56	0.40
1:B:516:LEU:HG	1:B:531:ILE:CD1	2.51	0.40
1:A:230:LEU:HD11	1:A:472:LEU:CD1	2.52	0.40
1:A:516:LEU:CD2	1:A:531:ILE:HD12	2.51	0.40
1:A:579:HIS:CD2	1:A:711:THR:OG1	2.75	0.40
1:A:735:ASP:H	1:A:737:LYS:HE3	1.86	0.40
1:A:740:LEU:HD22	1:A:740:LEU:O	2.22	0.40
1:B:119:GLY:CA	1:B:384:THR:HG21	2.50	0.40
1:B:579:HIS:CD2	1:B:711:THR:OG1	2.74	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	753/767 (98%)	723 (96%)	29 (4%)	1 (0%)	55	63
1	B	753/767 (98%)	722 (96%)	31 (4%)	0	100	100
All	All	1506/1534 (98%)	1445 (96%)	60 (4%)	1 (0%)	55	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	736	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	668/679 (98%)	622 (93%)	46 (7%)	18	19
1	B	668/679 (98%)	619 (93%)	49 (7%)	16	17
All	All	1336/1358 (98%)	1241 (93%)	95 (7%)	17	18

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1	MET
1	B	10	GLU
1	B	36	LEU
1	B	58	THR
1	B	70	LYS
1	B	71	ILE
1	B	92	GLU
1	B	118	THR
1	B	156	VAL
1	B	186	THR
1	B	197	LEU
1	B	222	LEU
1	B	224	THR
1	B	235	VAL
1	B	238	ARG
1	B	251	ASP
1	B	283	GLN
1	B	284	ARG
1	B	293	THR
1	B	311	THR
1	B	324	SER
1	B	384	THR
1	B	403	ASN

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Mol	Chain	Res	Type
1	B	406	ILE
1	B	407	ARG
1	B	408	VAL
1	B	412	LEU
1	B	427	ARG
1	B	460	SER
1	B	464	SER
1	B	489	GLU
1	B	507	GLU
1	B	510	LEU
1	B	543	LEU
1	B	551	VAL
1	B	608	LEU
1	B	623	LEU
1	B	662	LYS
1	B	686	VAL
1	B	687	LEU
1	B	699	PHE
1	B	702	THR
1	B	707	ILE
1	B	730	ASN
1	B	735	ASP
1	B	737	LYS
1	B	738	LEU
1	B	740	LEU
1	B	753	LEU
1	A	1	MET
1	A	10	GLU
1	A	36	LEU
1	A	58	THR
1	A	70	LYS
1	A	71	ILE
1	A	92	GLU
1	A	118	THR
1	A	156	VAL
1	A	186	THR
1	A	197	LEU
1	A	222	LEU
1	A	224	THR
1	A	235	VAL
1	A	238	ARG
1	A	251	ASP

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Mol	Chain	Res	Type
1	A	283	GLN
1	A	284	ARG
1	A	293	THR
1	A	311	THR
1	A	324	SER
1	A	384	THR
1	A	403	ASN
1	A	406	ILE
1	A	407	ARG
1	A	408	VAL
1	A	412	LEU
1	A	460	SER
1	A	464	SER
1	A	489	GLU
1	A	507	GLU
1	A	510	LEU
1	A	543	LEU
1	A	608	LEU
1	A	623	LEU
1	A	662	LYS
1	A	686	VAL
1	A	687	LEU
1	A	699	PHE
1	A	702	THR
1	A	707	ILE
1	A	730	ASN
1	A	737	LYS
1	A	738	LEU
1	A	740	LEU
1	A	753	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	54	GLN
1	B	260	ASN
1	B	283	GLN
1	B	296	GLN
1	B	298	HIS
1	B	353	GLN
1	B	403	ASN
1	B	422	GLN

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Mol	Chain	Res	Type
1	B	423	GLN
1	B	452	GLN
1	B	579	HIS
1	B	647	ASN
1	B	659	GLN
1	B	730	ASN
1	A	54	GLN
1	A	283	GLN
1	A	296	GLN
1	A	298	HIS
1	A	353	GLN
1	A	403	ASN
1	A	422	GLN
1	A	423	GLN
1	A	452	GLN
1	A	579	HIS
1	A	647	ASN
1	A	730	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 4 ligands modelled in this entry, 2 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	ADP	A	1000	2	25,29,29	1.37	4 (16%)	24,45,45	1.25	2 (8%)
3	ADP	B	1000	2	25,29,29	1.39	4 (16%)	24,45,45	1.22	3 (12%)

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	ADP	A	1000	2	-	0/12/32/32	0/3/3/3
3	ADP	B	1000	2	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1000	ADP	C2'-C1'	2.08	1.57	1.53
3	A	1000	ADP	C2'-C1'	2.16	1.57	1.53
3	B	1000	ADP	C2-N3	2.30	1.36	1.32
3	A	1000	ADP	C2-N3	2.38	1.36	1.32
3	B	1000	ADP	C5-C4	3.07	1.47	1.40
3	A	1000	ADP	C5-C4	3.23	1.47	1.40
3	B	1000	ADP	O4'-C1'	3.84	1.46	1.41
3	A	1000	ADP	O4'-C1'	3.89	1.46	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	ADP	O5'-C5'-C4'	-2.83	98.97	109.00
3	B	1000	ADP	O5'-C5'-C4'	-2.77	99.19	109.00
3	B	1000	ADP	O4'-C4'-C3'	2.25	109.64	105.17
3	B	1000	ADP	N3-C2-N1	2.54	131.07	128.86
3	A	1000	ADP	N3-C2-N1	2.64	131.16	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	ADP	2	0
3	B	1000	ADP	3	0

## 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	755/767 (98%)	0.17	42 (5%)	25 24	23, 48, 100, 191	0
1	B	755/767 (98%)	0.00	25 (3%)	47 44	22, 44, 100, 191	0
All	All	1510/1534 (98%)	0.09	67 (4%)	35 33	22, 46, 100, 191	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	13.9
1	A	1	MET	13.6
1	B	755	GLN	9.8
1	B	754	LYS	9.6
1	A	754	LYS	8.3
1	A	753	LEU	7.7
1	A	755	GLN	7.2
1	B	668	LYS	5.8
1	B	735	ASP	5.6
1	B	751	ASN	5.4
1	A	734	GLY	5.3
1	B	405	ARG	4.4
1	A	690	ASP	4.4
1	A	404	PRO	4.4
1	A	733	LYS	4.3
1	B	733	LYS	4.3
1	A	735	ASP	4.0
1	A	748	ASP	3.9
1	A	252	ALA	3.9
1	B	753	LEU	3.8
1	B	702	THR	3.7
1	A	689	HIS	3.5
1	B	732	GLN	3.4
1	A	669	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	732	GLN	3.4
1	A	668	LYS	3.4
1	B	2	GLY	3.3
1	B	734	GLY	3.2
1	A	34	HIS	3.2
1	A	250	LEU	3.2
1	B	747	VAL	3.1
1	A	2	GLY	3.1
1	A	740	LEU	3.1
1	B	406	ILE	3.0
1	A	405	ARG	3.0
1	B	407	ARG	3.0
1	A	751	ASN	3.0
1	A	559	THR	2.9
1	B	250	LEU	2.9
1	B	252	ALA	2.7
1	A	749	ARG	2.7
1	A	595	TYR	2.7
1	B	749	ARG	2.6
1	A	63	ALA	2.6
1	B	741	GLU	2.6
1	A	78	GLU	2.6
1	B	750	LEU	2.4
1	A	35	PRO	2.4
1	B	746	LYS	2.3
1	A	687	LEU	2.3
1	A	253	GLU	2.3
1	A	83	TYR	2.3
1	B	378	ILE	2.3
1	A	752	GLU	2.2
1	A	572	PHE	2.2
1	A	43	VAL	2.2
1	A	53	LEU	2.2
1	A	76	GLY	2.2
1	A	699	PHE	2.1
1	B	151	VAL	2.1
1	A	47	ALA	2.1
1	A	257	ARG	2.1
1	A	92	GLU	2.1
1	A	70	LYS	2.1
1	A	376	THR	2.0
1	B	596	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	592	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. 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	ADP	B	1000	27/27	0.95	0.19	1.32	23,54,71,84	0
2	MG	A	800	1/1	0.98	0.19	0.84	31,31,31,31	0
2	MG	B	800	1/1	0.96	0.18	0.82	32,32,32,32	0
3	ADP	A	1000	27/27	0.95	0.16	0.54	26,50,70,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.