



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:05 PM GMT

PDB ID : 4USJ  
Title : N-acetylglutamate kinase from Arabidopsis thaliana in complex with PII from Chlamydomonas reinhardtii  
Authors : Chellamuthu, V.R.; Forchhammer, K.; Hartmann, M.D.  
Deposited on : 2014-07-08  
Resolution : 2.85 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

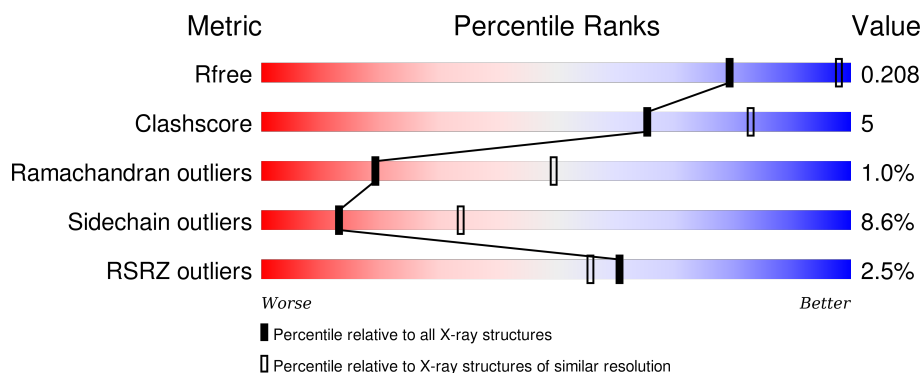
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	318	<div> <div>3%</div> <div>70% 16% • 12%</div> </div>
1	B	318	<div> <div>3%</div> <div>70% 15% • 12%</div> </div>
2	C	154	<div> <div>85% 6% • 8%</div> </div>
2	D	154	<div> <div>2%</div> <div>84% 6% • 8%</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	ARG	A	301	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6567 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 ACETYLGLUTAMATE KINASE, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2066	1304	359	393	10			
1	B	281	Total	C	N	O	S	0	0	0
			2058	1298	357	393	10			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q9SCL7
A	-19	GLY	-	EXPRESSION TAG	UNP Q9SCL7
A	-18	SER	-	EXPRESSION TAG	UNP Q9SCL7
A	-17	SER	-	EXPRESSION TAG	UNP Q9SCL7
A	-16	HIS	-	EXPRESSION TAG	UNP Q9SCL7
A	-15	HIS	-	EXPRESSION TAG	UNP Q9SCL7
A	-14	HIS	-	EXPRESSION TAG	UNP Q9SCL7
A	-13	HIS	-	EXPRESSION TAG	UNP Q9SCL7
A	-12	HIS	-	EXPRESSION TAG	UNP Q9SCL7
A	-11	HIS	-	EXPRESSION TAG	UNP Q9SCL7
A	-10	SER	-	EXPRESSION TAG	UNP Q9SCL7
A	-9	SER	-	EXPRESSION TAG	UNP Q9SCL7
A	-8	GLY	-	EXPRESSION TAG	UNP Q9SCL7
A	-7	LEU	-	EXPRESSION TAG	UNP Q9SCL7
A	-6	VAL	-	EXPRESSION TAG	UNP Q9SCL7
A	-5	PRO	-	EXPRESSION TAG	UNP Q9SCL7
A	-4	ARG	-	EXPRESSION TAG	UNP Q9SCL7
A	-3	GLY	-	EXPRESSION TAG	UNP Q9SCL7
A	-2	SER	-	EXPRESSION TAG	UNP Q9SCL7
A	-1	HIS	-	EXPRESSION TAG	UNP Q9SCL7
A	0	MET	-	EXPRESSION TAG	UNP Q9SCL7
B	-20	MET	-	EXPRESSION TAG	UNP Q9SCL7
B	-19	GLY	-	EXPRESSION TAG	UNP Q9SCL7
B	-18	SER	-	EXPRESSION TAG	UNP Q9SCL7
B	-17	SER	-	EXPRESSION TAG	UNP Q9SCL7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	EXPRESSION TAG	UNP Q9SCL7
B	-15	HIS	-	EXPRESSION TAG	UNP Q9SCL7
B	-14	HIS	-	EXPRESSION TAG	UNP Q9SCL7
B	-13	HIS	-	EXPRESSION TAG	UNP Q9SCL7
B	-12	HIS	-	EXPRESSION TAG	UNP Q9SCL7
B	-11	HIS	-	EXPRESSION TAG	UNP Q9SCL7
B	-10	SER	-	EXPRESSION TAG	UNP Q9SCL7
B	-9	SER	-	EXPRESSION TAG	UNP Q9SCL7
B	-8	GLY	-	EXPRESSION TAG	UNP Q9SCL7
B	-7	LEU	-	EXPRESSION TAG	UNP Q9SCL7
B	-6	VAL	-	EXPRESSION TAG	UNP Q9SCL7
B	-5	PRO	-	EXPRESSION TAG	UNP Q9SCL7
B	-4	ARG	-	EXPRESSION TAG	UNP Q9SCL7
B	-3	GLY	-	EXPRESSION TAG	UNP Q9SCL7
B	-2	SER	-	EXPRESSION TAG	UNP Q9SCL7
B	-1	HIS	-	EXPRESSION TAG	UNP Q9SCL7
B	0	MET	-	EXPRESSION TAG	UNP Q9SCL7

- Molecule 2 is a protein called NITROGEN REGULATORY PROTEIN PII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	142	Total	C	N	O	S	0	1	0
			1087	694	188	200	5			
2	D	142	Total	C	N	O	S	0	1	0
			1086	694	187	200	5			

There are 22 discrepancies between the modelled and reference sequences:

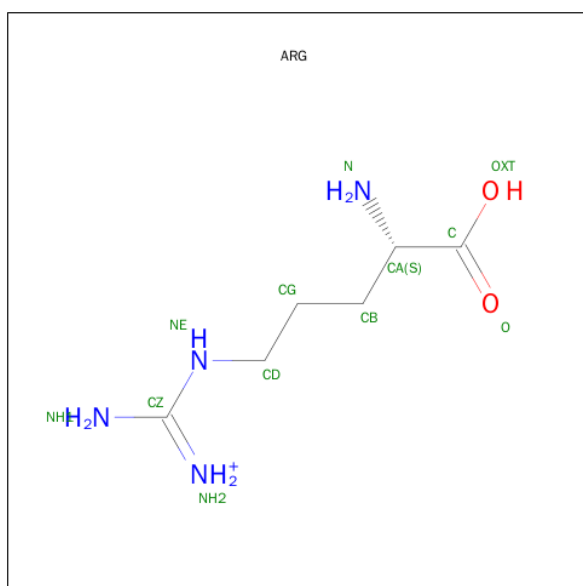
Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	EXPRESSION TAG	UNP A8JI83
C	145	SER	-	EXPRESSION TAG	UNP A8JI83
C	146	ALA	-	EXPRESSION TAG	UNP A8JI83
C	147	TRP	-	EXPRESSION TAG	UNP A8JI83
C	148	SER	-	EXPRESSION TAG	UNP A8JI83
C	149	HIS	-	EXPRESSION TAG	UNP A8JI83
C	150	PRO	-	EXPRESSION TAG	UNP A8JI83
C	151	GLN	-	EXPRESSION TAG	UNP A8JI83
C	152	PHE	-	EXPRESSION TAG	UNP A8JI83
C	153	GLU	-	EXPRESSION TAG	UNP A8JI83
C	154	LYS	-	EXPRESSION TAG	UNP A8JI83
D	1	MET	-	EXPRESSION TAG	UNP A8JI83
D	145	SER	-	EXPRESSION TAG	UNP A8JI83

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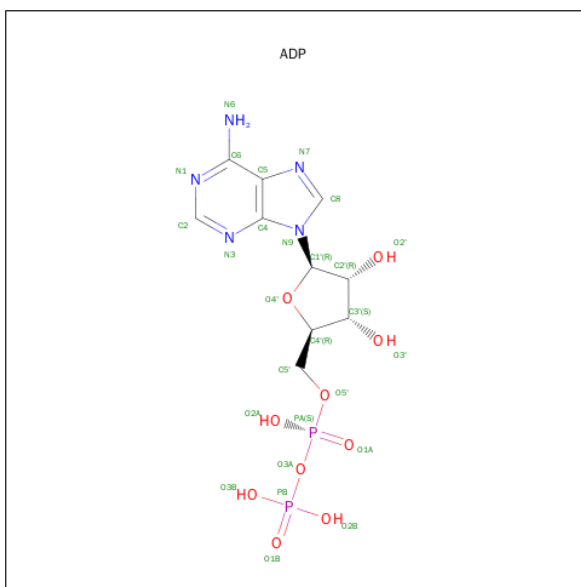
Chain	Residue	Modelled	Actual	Comment	Reference
D	146	ALA	-	EXPRESSION TAG	UNP A8JI83
D	147	TRP	-	EXPRESSION TAG	UNP A8JI83
D	148	SER	-	EXPRESSION TAG	UNP A8JI83
D	149	HIS	-	EXPRESSION TAG	UNP A8JI83
D	150	PRO	-	EXPRESSION TAG	UNP A8JI83
D	151	GLN	-	EXPRESSION TAG	UNP A8JI83
D	152	PHE	-	EXPRESSION TAG	UNP A8JI83
D	153	GLU	-	EXPRESSION TAG	UNP A8JI83
D	154	LYS	-	EXPRESSION TAG	UNP A8JI83

- Molecule 3 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



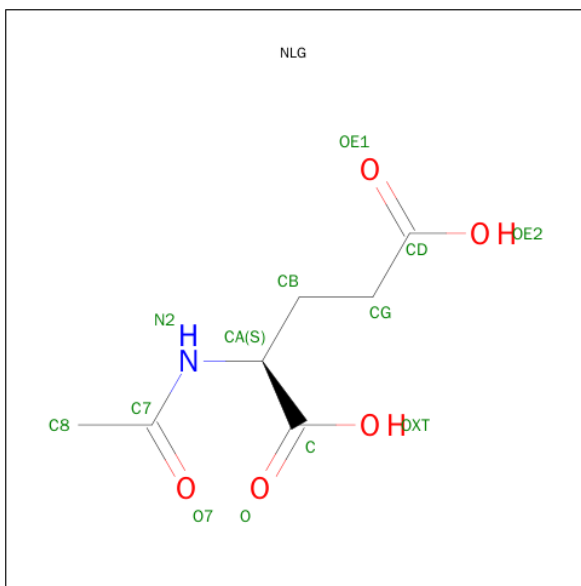
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	6	4	2		
3	B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 5 is N-ACETYL-L-GLUTAMATE (three-letter code: NLG) (formula:  $C_7H_{11}NO_5$ ).

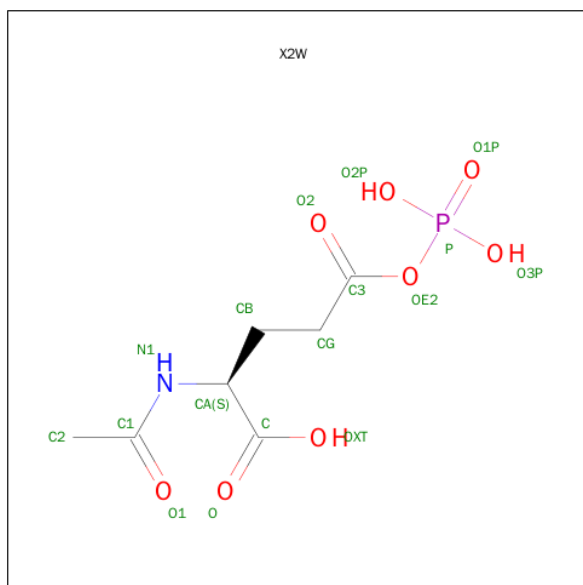


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O		
			13	7	1	5		
							0	
								0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

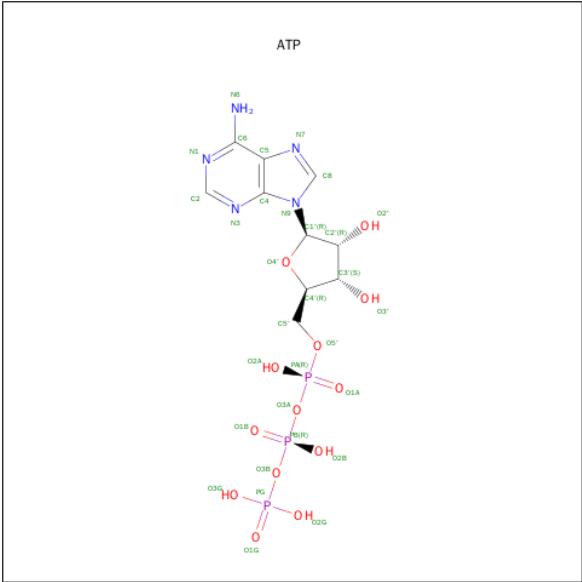
- Molecule 7 is N-ACETYL-L-GLUTAMYL 5-PHOSPHATE (three-letter code: X2W) (formula:  $C_7H_{12}NO_8P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O P 17 7 1 8 1	0	0

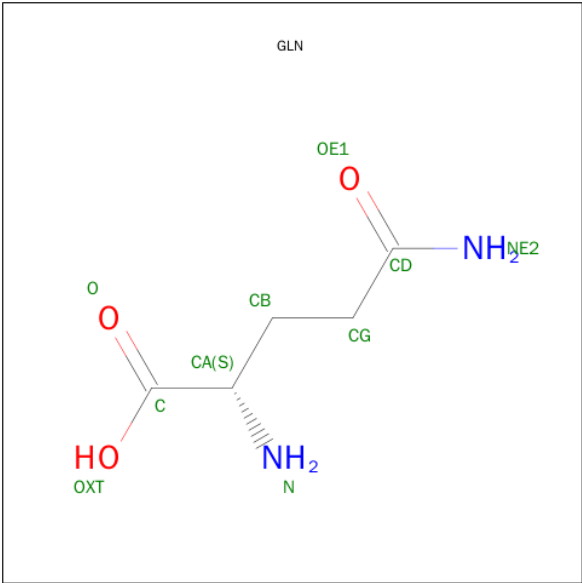
- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).





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

- Molecule 9 is GLUTAMINE (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).



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

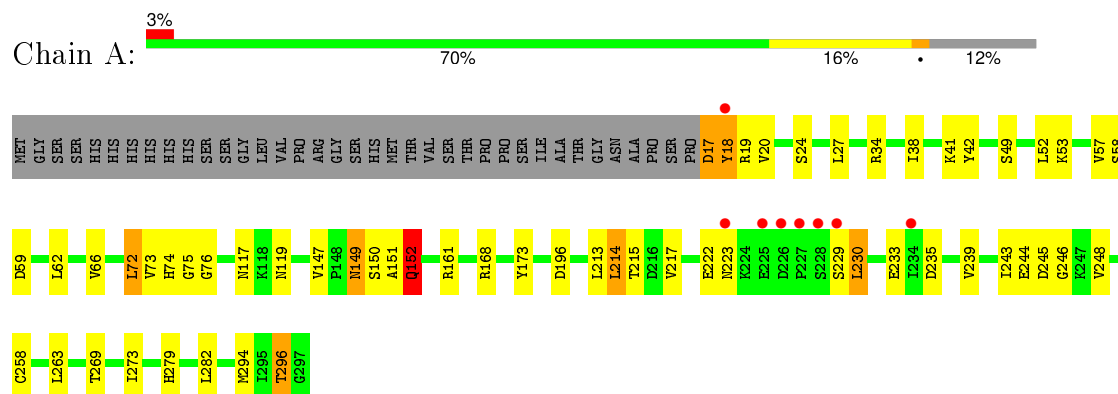
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	37	Total 37	O 37	0	0
10	B	30	Total 30	O 30	0	0
10	C	20	Total 20	O 20	0	0
10	D	17	Total 17	O 17	0	0

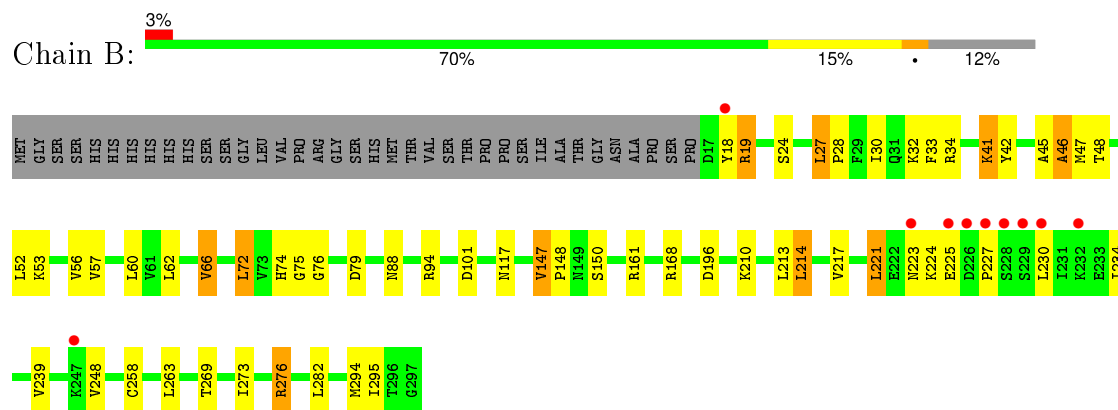
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $RSRZ > 2$ ). 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.

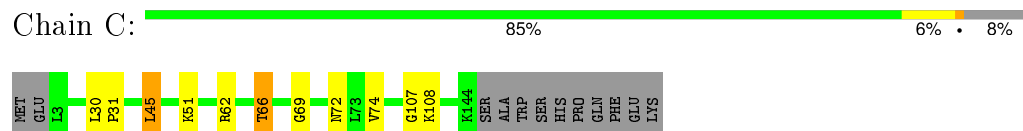
#### • Molecule 1: ACETYLGLUTAMATE KINASE, CHLOROPLASTIC



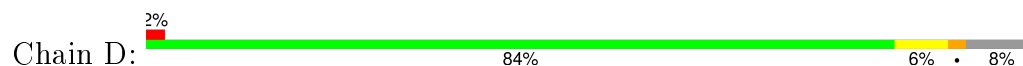
#### • Molecule 1: ACETYLGLUTAMATE KINASE, CHLOROPLASTIC

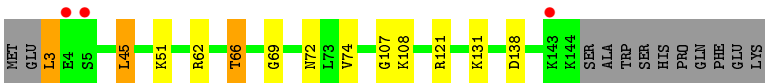


#### • Molecule 2: NITROGEN REGULATORY PROTEIN PII



#### • Molecule 2: NITROGEN REGULATORY PROTEIN PII





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.43Å 171.43Å 171.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.36 – 2.85 39.33 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.36-2.85) 99.2 (39.33-2.85)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.189 , 0.220 0.173 , 0.208	Depositor DCC
$R_{free}$ test set	2027 reflections (5.47%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.4	EDS
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 39062 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: ATP, MG, X2W, ADP, NLG

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	0.83	0/2091	0.98	4/2832 (0.1%)
1	B	0.78	0/2083	0.96	5/2824 (0.2%)
2	C	0.75	0/1109	0.92	2/1496 (0.1%)
2	D	0.77	0/1108	0.95	5/1495 (0.3%)
All	All	0.79	0/6391	0.96	16/8647 (0.2%)

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	A	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	ASP	CB-CG-OD1	5.95	123.65	118.30
2	D	3	LEU	CA-CB-CG	5.92	128.91	115.30
2	D	62	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	214	LEU	CA-CB-CG	5.84	128.73	115.30
1	B	19	ARG	NE-CZ-NH1	5.79	123.20	120.30
2	C	62	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	152	GLN	CB-CA-C	-5.35	99.70	110.40
1	B	94	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	196	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	276	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	D	45	LEU	CA-CB-CG	5.22	127.31	115.30
2	C	45	LEU	CA-CB-CG	5.21	127.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	LEU	CA-CB-CG	5.20	127.26	115.30
2	D	62	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	94	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	D	121	ARG	NE-CZ-NH1	5.09	122.85	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	SER	Peptide

## 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	2066	0	2153	26	0
1	B	2058	0	2131	27	0
2	C	1087	0	1096	7	0
2	D	1086	0	1091	7	0
3	A	12	0	12	0	0
3	B	12	0	12	2	0
4	A	27	0	12	0	0
5	A	13	0	9	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	B	17	0	9	0	0
8	C	31	0	12	2	0
8	D	31	0	12	2	0
9	C	10	0	7	0	0
9	D	10	0	7	0	0
10	A	37	0	0	0	0
10	B	30	0	0	1	0
10	C	20	0	0	0	0
10	D	17	0	0	0	0
All	All	6567	0	6563	65	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 5.

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ARG:HA	2:C:66:THR:HB	1.68	0.76
2:C:69:GLY:H	2:C:72:ASN:HD22	1.31	0.76
1:A:161:ARG:HA	2:D:66:THR:HB	1.68	0.74
2:D:69:GLY:H	2:D:72:ASN:HD22	1.37	0.73
1:A:74:HIS:HE1	1:A:117:ASN:HD22	1.36	0.71
1:A:149:ASN:HD22	1:A:149:ASN:H	1.43	0.66
1:A:269:THR:HB	1:A:294:MET:HE2	1.78	0.64
1:B:217:VAL:HA	1:B:276:ARG:HH21	1.63	0.64
1:B:41:LYS:HD2	1:B:196:ASP:OD1	1.97	0.64
1:B:74:HIS:HE1	1:B:117:ASN:HD22	1.46	0.62
2:C:69:GLY:N	2:C:72:ASN:HD22	1.98	0.61
1:A:17:ASP:OD1	1:A:18:TYR:N	2.33	0.61
2:D:69:GLY:N	2:D:72:ASN:HD22	1.99	0.60
2:C:69:GLY:H	2:C:72:ASN:ND2	2.02	0.56
1:B:74:HIS:HD2	1:B:75:GLY:O	1.88	0.56
1:A:214:LEU:HD22	1:A:273:ILE:HD11	1.86	0.56
1:B:234:ILE:O	1:B:295:ILE:HA	2.06	0.55
1:A:269:THR:HB	1:A:294:MET:CE	2.36	0.55
1:B:30:ILE:HG23	1:B:66:VAL:HG13	1.89	0.55
1:A:17:ASP:C	1:A:17:ASP:OD1	2.46	0.54
1:A:74:HIS:HD2	1:A:75:GLY:O	1.92	0.53
1:A:269:THR:CG2	1:A:294:MET:HE2	2.39	0.53
1:B:214:LEU:HD22	1:B:273:ILE:HD11	1.90	0.52
2:D:131:LYS:NZ	2:D:138:ASP:OD1	2.40	0.51
1:A:62:LEU:HD23	1:A:282:LEU:HD11	1.93	0.51
1:A:149:ASN:O	1:A:152:GLN:HG2	2.11	0.51
1:B:210:LYS:HE3	3:B:301:ARG:OXT	2.11	0.50
1:A:269:THR:CB	1:A:294:MET:HE2	2.41	0.50
1:A:42:TYR:OH	1:A:53:LYS:HA	2.10	0.50
1:B:45:ALA:O	1:B:47:MET:N	2.45	0.50
2:C:108:LYS:HE3	8:C:301:ATP:O1B	2.11	0.50
1:B:32:LYS:HD3	10:B:2002:HOH:O	2.11	0.50
1:A:243:ILE:HG12	1:A:248:VAL:HG22	1.94	0.49
1:A:149:ASN:HB2	1:A:152:GLN:HG2	1.94	0.49
1:B:41:LYS:HB3	1:B:213:LEU:HD23	1.94	0.48
1:A:41:LYS:HA	1:A:73:VAL:O	2.13	0.48
2:D:69:GLY:H	2:D:72:ASN:ND2	2.07	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:LYS:HE3	8:D:301:ATP:O1B	2.14	0.47
1:A:42:TYR:HB2	1:A:72:LEU:HD21	1.96	0.47
1:B:60:LEU:HD11	1:B:72:LEU:HG	1.97	0.47
1:B:294:MET:HB2	3:B:301:ARG:NH1	2.30	0.46
1:A:53:LYS:NZ	1:A:119:ASN:HD21	2.14	0.46
2:D:107:GLY:HA2	8:D:301:ATP:H5'1	1.95	0.46
1:A:222:GLU:HB3	1:A:229:SER:HB2	1.97	0.46
1:B:52:LEU:O	1:B:56:VAL:HG23	2.16	0.46
1:B:45:ALA:O	1:B:46:ALA:C	2.56	0.44
1:A:41:LYS:HB3	1:A:213:LEU:HD23	2.00	0.43
2:C:107:GLY:HA2	8:C:301:ATP:H5'1	1.99	0.43
1:B:32:LYS:HG2	1:B:33:PHE:CZ	2.54	0.43
1:B:223:ASN:HD21	1:B:225:GLU:HG2	1.84	0.42
1:B:221:LEU:CD2	1:B:227:PRO:HA	2.49	0.42
1:B:42:TYR:OH	1:B:53:LYS:HA	2.18	0.42
1:B:269:THR:CG2	1:B:294:MET:HE2	2.49	0.42
1:B:269:THR:HB	1:B:294:MET:HE2	2.02	0.42
1:B:45:ALA:C	1:B:47:MET:N	2.73	0.41
1:A:59:ASP:OD2	1:A:279:HIS:HA	2.19	0.41
1:B:27:LEU:N	1:B:28:PRO:CD	2.84	0.41
1:B:62:LEU:HD23	1:B:282:LEU:HD11	2.03	0.41
1:A:244:GLU:O	1:A:246:GLY:N	2.54	0.41
1:A:215:THR:HG23	1:A:217:VAL:H	1.86	0.41
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.74	0.40
1:B:147:VAL:HG22	1:B:148:PRO:HD2	2.02	0.40
1:A:282:LEU:HA	1:A:282:LEU:HD23	1.90	0.40
2:C:30:LEU:HB3	2:C:31:PRO:HD3	2.04	0.40
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.93	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	279/318 (88%)	261 (94%)	13 (5%)	5 (2%)	11	33
1	B	279/318 (88%)	262 (94%)	14 (5%)	3 (1%)	17	47
2	C	141/154 (92%)	135 (96%)	6 (4%)	0	100	100
2	D	141/154 (92%)	134 (95%)	7 (5%)	0	100	100
All	All	840/944 (89%)	792 (94%)	40 (5%)	8 (1%)	19	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ALA
1	B	46	ALA
1	A	245	ASP
1	B	19	ARG
1	A	76	GLY
1	A	173	TYR
1	A	296	THR
1	B	76	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	223/256 (87%)	198 (89%)	25 (11%)	7	20
1	B	221/256 (86%)	199 (90%)	22 (10%)	9	26
2	C	113/127 (89%)	109 (96%)	4 (4%)	43	76
2	D	112/127 (88%)	107 (96%)	5 (4%)	34	67
All	All	669/766 (87%)	613 (92%)	56 (8%)	13	35

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	18	TYR
1	A	19	ARG

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Mol	Chain	Res	Type
1	A	20	VAL
1	A	24	SER
1	A	27	LEU
1	A	34	ARG
1	A	38	ILE
1	A	49	SER
1	A	57	VAL
1	A	58	SER
1	A	66	VAL
1	A	72	LEU
1	A	147	VAL
1	A	149	ASN
1	A	152	GLN
1	A	168	ARG
1	A	223	ASN
1	A	230	LEU
1	A	233	GLU
1	A	235	ASP
1	A	239	VAL
1	A	258	CYS
1	A	263	LEU
1	A	296	THR
1	B	18	TYR
1	B	24	SER
1	B	27	LEU
1	B	34	ARG
1	B	41	LYS
1	B	48	THR
1	B	57	VAL
1	B	66	VAL
1	B	72	LEU
1	B	79	ASP
1	B	88	ASN
1	B	147	VAL
1	B	150	SER
1	B	168	ARG
1	B	214	LEU
1	B	221	LEU
1	B	224	LYS
1	B	230	LEU
1	B	239	VAL
1	B	248	VAL

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Mol	Chain	Res	Type
1	B	258	CYS
1	B	263	LEU
2	C	45	LEU
2	C	51	LYS
2	C	66	THR
2	C	74	VAL
2	D	3	LEU
2	D	45	LEU
2	D	51	LYS
2	D	66	THR
2	D	74	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	119	ASN
1	A	149	ASN
1	B	74	HIS
1	B	119	ASN
1	B	223	ASN
2	C	47	ASN
2	C	72	ASN
2	C	87	GLN
2	D	47	ASN
2	D	72	ASN
2	D	87	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 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	ARG	A	301	-	5,11,11	0.43	0	3,13,13	1.04	0
4	ADP	A	302	6	22,29,29	1.19	1 (4%)	27,45,45	2.69	6 (22%)
5	NLG	A	303	-	6,12,12	1.23	1 (16%)	5,15,15	0.60	0
3	ARG	B	301	-	5,11,11	0.45	0	3,13,13	0.50	0
7	X2W	B	303	-	11,16,16	1.30	1 (9%)	12,22,22	1.53	2 (16%)
8	ATP	C	301	6	24,33,33	0.94	2 (8%)	31,52,52	2.19	8 (25%)
9	GLN	C	303	-	6,9,9	0.40	0	5,11,11	0.37	0
8	ATP	D	301	6	24,33,33	1.15	1 (4%)	31,52,52	1.98	6 (19%)
9	GLN	D	303	-	6,9,9	0.34	0	5,11,11	0.35	0

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	ARG	A	301	-	-	0/5/11/11	0/0/0/0
4	ADP	A	302	6	-	0/12/32/32	0/3/3/3
5	NLG	A	303	-	-	0/7/13/13	0/0/0/0
3	ARG	B	301	-	-	0/5/11/11	0/0/0/0
7	X2W	B	303	-	-	0/12/18/18	0/0/0/0
8	ATP	C	301	6	-	0/18/38/38	0/3/3/3
9	GLN	C	303	-	-	0/5/9/9	0/0/0/0
8	ATP	D	301	6	-	0/18/38/38	0/3/3/3
9	GLN	D	303	-	-	0/5/9/9	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	303	NLG	CA-N2	-2.52	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	301	ATP	C5-N7	-2.02	1.32	1.39
8	C	301	ATP	C5-C4	2.59	1.46	1.40
8	D	301	ATP	C5-C4	2.95	1.47	1.40
7	B	303	X2W	CB-CA	3.37	1.58	1.53
4	A	302	ADP	C5-C4	3.73	1.48	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	302	ADP	N3-C2-N1	-8.59	122.32	128.89
4	A	302	ADP	O3A-PA-O5'	-7.49	83.06	102.94
8	C	301	ATP	N3-C2-N1	-7.16	123.41	128.89
8	D	301	ATP	N3-C2-N1	-5.12	124.98	128.89
8	D	301	ATP	C4-C5-N7	-4.81	105.06	109.48
8	C	301	ATP	C4-C5-N7	-4.59	105.25	109.48
8	C	301	ATP	PA-O3A-PB	-3.45	123.04	132.73
8	C	301	ATP	O3A-PA-O5'	-3.37	93.99	102.94
8	C	301	ATP	PB-O3B-PG	-3.25	121.75	132.67
8	D	301	ATP	PB-O3B-PG	-3.10	122.28	132.67
8	D	301	ATP	PA-O3A-PB	-2.99	124.32	132.73
7	B	303	X2W	O2-C3-CG	-2.99	111.77	123.72
8	C	301	ATP	O4'-C1'-N9	-2.71	102.42	108.10
8	C	301	ATP	C1'-N9-C4	-2.51	123.15	126.94
4	A	302	ADP	C2'-C1'-N9	2.19	117.63	114.29
7	B	303	X2W	CB-CG-C3	2.24	119.88	113.32
4	A	302	ADP	C2-N1-C6	2.77	123.71	118.77
8	C	301	ATP	C2-N1-C6	2.91	123.97	118.77
4	A	302	ADP	O2B-PB-O1B	2.95	120.07	110.58
8	D	301	ATP	O3G-PG-O2G	2.97	118.70	107.38
8	D	301	ATP	O2B-PB-O3A	4.48	125.43	105.09
4	A	302	ADP	O5'-PA-O1A	4.76	128.08	109.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	ARG	2	0
8	C	301	ATP	2	0
8	D	301	ATP	2	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	281/318 (88%)	-0.24	8 (2%) 56 51	36, 53, 89, 132	0
1	B	281/318 (88%)	-0.23	10 (3%) 46 39	38, 56, 110, 143	0
2	C	142/154 (92%)	-0.32	0 100 100	40, 58, 80, 102	0
2	D	142/154 (92%)	-0.20	3 (2%) 67 62	39, 56, 76, 115	0
All	All	846/944 (89%)	-0.24	21 (2%) 61 56	36, 56, 98, 143	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	GLU	5.3
1	B	18	TYR	3.7
1	B	227	PRO	3.5
1	B	226	ASP	3.5
2	D	143	LYS	3.0
2	D	5	SER	2.9
1	B	228	SER	2.8
1	B	223	ASN	2.8
1	B	229	SER	2.8
1	A	228	SER	2.7
1	B	232	LYS	2.6
1	A	226	ASP	2.4
1	A	18	TYR	2.4
1	A	225	GLU	2.4
1	A	234	ILE	2.3
1	B	230	LEU	2.2
1	B	247	LYS	2.1
1	A	223	ASN	2.1
1	A	227	PRO	2.1
1	A	229	SER	2.1
2	D	4	GLU	2.1



## 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	ARG	A	301	12/12	0.96	0.23	2.19	66,68,71,77	0
7	X2W	B	303	17/17	0.92	0.19	0.60	47,51,102,105	0
3	ARG	B	301	12/12	0.96	0.24	0.53	69,75,86,86	0
9	GLN	D	303	10/10	0.93	0.18	0.09	44,59,71,80	0
9	GLN	C	303	10/10	0.93	0.18	0.02	54,62,76,82	0
5	NLG	A	303	13/13	0.97	0.17	-0.33	40,45,49,50	0
4	ADP	A	302	27/27	0.96	0.14	-0.56	45,59,63,64	0
8	ATP	D	301	31/31	0.97	0.14	-0.75	41,48,52,54	0
8	ATP	C	301	31/31	0.98	0.11	-1.43	42,48,52,56	0
6	MG	D	302	1/1	0.98	0.05	-3.79	53,53,53,53	0
6	MG	C	302	1/1	0.97	0.04	-4.09	58,58,58,58	0
6	MG	A	304	1/1	0.96	0.23	-	41,41,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.