Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:36 AM GMT

PDB ID	:	2RD5
Title	:	Structural basis for the regulation of N-acetylglutamate kinase by PII in Arabidopsis thaliana
Authors	:	Mizuno, Y.; Moorhead, G.B.G.; Ng, K.K.S.
Deposited on	:	2007-09-21
Resolution	:	2.51 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

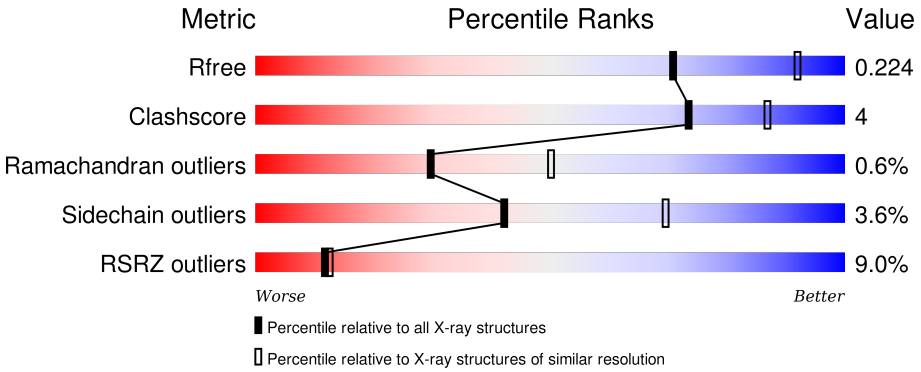
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	3553 (2.50-2.50)
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 >=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 <=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	298	6% 82% 11% • 6%
1	B	298	9% 84% 11% 5%
2	C	135	12% 85% 7% 7%
2	D	135	10% 81% 12% • 7%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6328 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-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2074	1309	360	395	10			
1	B	283	Total	C	N	O	S	0	0	0
			2087	1317	362	398	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING METHIONINE	UNP Q9SCL7
B	0	MET	-	INITIATING METHIONINE	UNP Q9SCL7

- Molecule 2 is a protein called PII protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	125	Total	C	N	O	S	0	0	0
			963	605	171	185	2			
2	D	126	Total	C	N	O	S	0	0	0
			971	610	172	186	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	INITIATING METHIONINE	UNP Q9ZST4
D	0	MET	-	INITIATING METHIONINE	UNP Q9ZST4

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

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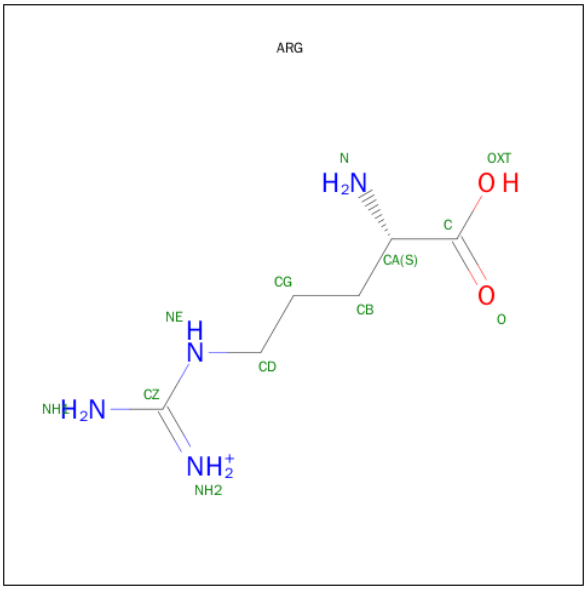
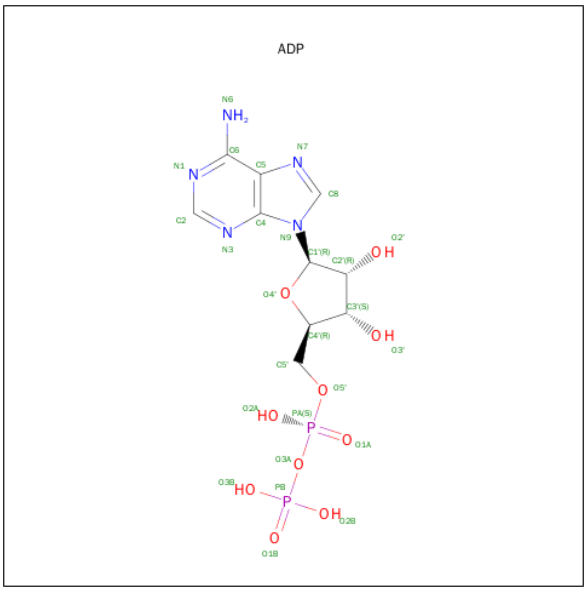
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



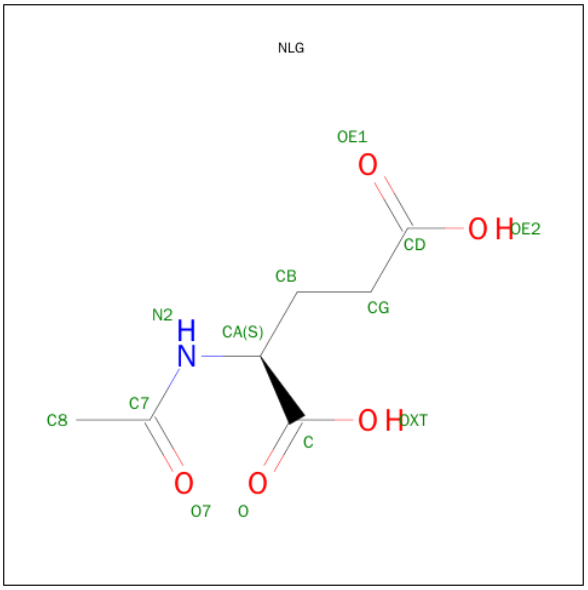
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 12 6 4 2	0	0
4	B	1	Total C N O 12 6 4 2	0	0

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



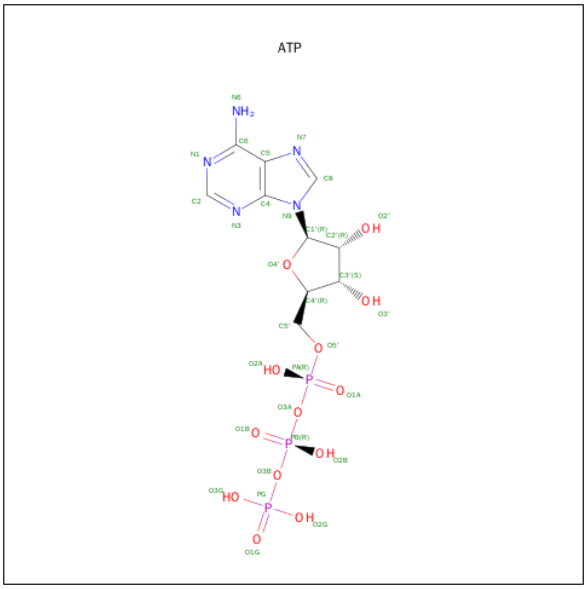
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is N-ACETYL-L-GLUTAMATE (three-letter code: NLG) (formula: $C_7H_{11}NO_5$).



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

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 8 is water.

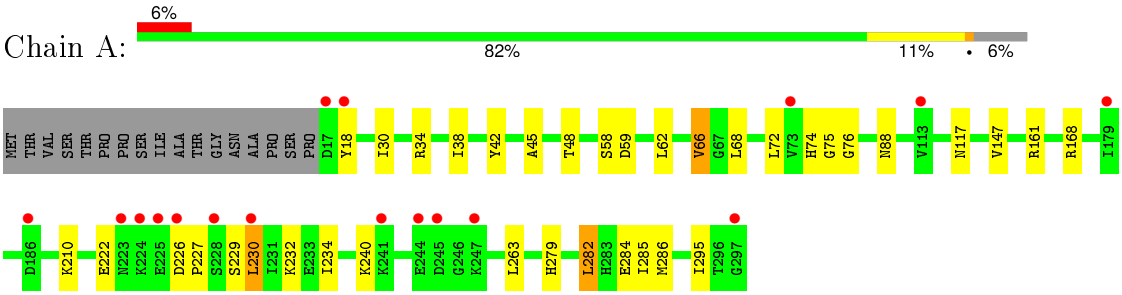
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	24	Total	O	0	0
			24	24		
8	B	25	Total	O	0	0
			25	25		
8	C	4	Total	O	0	0
			4	4		
8	D	11	Total	O	0	0
			11	11		

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.

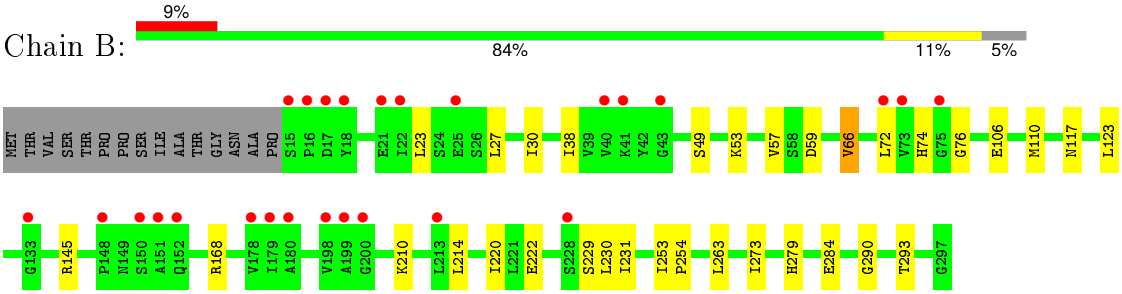
- Molecule 1: Acetylglutamate kinase-like protein

Chain A:



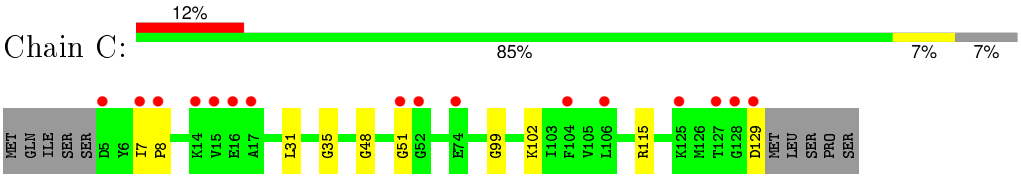
- Molecule 1: Acetylglutamate kinase-like protein

Chain B:



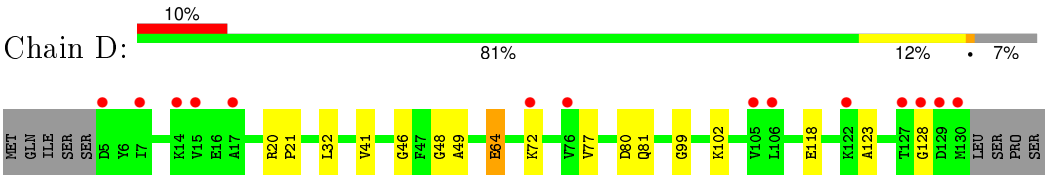
- Molecule 2: PII protein

Chain C:



- Molecule 2: PII protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	171.13Å 171.13Å 171.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.51 32.93 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.51) 99.9 (32.93-2.51)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	3.23 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.229 0.197 , 0.224	Depositor DCC
R_{free} test set	2900 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	49.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.3	EDS
Estimated twinning fraction	0.031 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 57272 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6328	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, ADP, 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	0.38	0/2099	0.55	1/2841 (0.0%)
1	B	0.38	0/2113	0.57	0/2861
2	C	0.41	0/975	0.55	0/1307
2	D	0.39	0/983	0.57	0/1317
All	All	0.39	0/6170	0.56	1/8326 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	230	LEU	CA-CB-CG	5.25	127.38	115.30

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	2074	0	2168	20	0
1	B	2087	0	2180	14	0
2	C	963	0	985	6	1
2	D	971	0	994	10	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	12	0	12	2	0
4	B	12	0	12	0	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
6	A	13	0	8	0	0
6	B	13	0	8	0	0
7	C	31	0	12	4	1
7	D	31	0	12	5	0
8	A	24	0	0	0	0
8	B	25	0	0	0	0
8	C	4	0	0	1	0
8	D	11	0	0	2	0
All	All	6328	0	6415	52	1

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 4.

All (52) 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)
2:C:7:ILE:HG23	2:C:8:PRO:HD3	1.40	1.03
2:D:48:GLY:HA3	7:D:1000:ATP:O1A	1.66	0.94
1:A:74:HIS:HE1	1:A:117:ASN:HD22	1.16	0.92
2:C:48:GLY:HA3	7:C:1000:ATP:O1A	1.70	0.91
1:A:38:ILE:HD12	1:A:68:LEU:HD23	1.55	0.87
1:B:74:HIS:HE1	1:B:117:ASN:HD22	1.22	0.81
1:B:30:ILE:HG23	1:B:66:VAL:HG13	1.70	0.72
1:A:30:ILE:HG23	1:A:66:VAL:HG13	1.73	0.70
1:B:106:GLU:O	1:B:110:MET:HG2	1.93	0.67
1:B:222:GLU:HB2	1:B:231:ILE:HD11	1.77	0.66
2:D:99:GLY:HA2	7:D:1000:ATP:O2A	1.96	0.65
2:C:99:GLY:HA2	7:C:1000:ATP:O2A	1.98	0.63
1:A:285:ILE:HG22	1:A:286:MET:CE	2.30	0.61
1:A:74:HIS:CE1	1:A:117:ASN:HD22	2.08	0.59
2:C:7:ILE:CG2	2:C:8:PRO:HD3	2.24	0.57
2:D:77:VAL:HB	2:D:81:GLN:HG3	1.88	0.55
1:A:38:ILE:HG12	1:A:210:LYS:HB2	1.90	0.53
1:B:59:ASP:OD1	1:B:279:HIS:HD2	1.91	0.53
2:D:49:ALA:CB	2:D:64:GLU:HA	2.38	0.53
1:B:222:GLU:HB3	1:B:229:SER:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ILE:HG22	1:A:286:MET:HE3	1.91	0.53
1:A:232:LYS:O	4:A:1000:ARG:NH2	2.44	0.51
2:D:102:LYS:HG3	7:D:1000:ATP:C8	2.46	0.51
1:A:285:ILE:HG22	1:A:286:MET:HE2	1.93	0.51
1:A:42:TYR:HB2	1:A:72:LEU:HD21	1.92	0.50
1:A:222:GLU:HB3	1:A:229:SER:HB2	1.93	0.49
1:B:253:ILE:HB	1:B:254:PRO:HD3	1.94	0.49
1:A:62:LEU:HD23	1:A:282:LEU:HD21	1.96	0.48
1:A:59:ASP:OD1	1:A:279:HIS:HD2	1.97	0.48
1:A:45:ALA:HA	1:A:48:THR:HG22	1.97	0.47
1:B:214:LEU:HD22	1:B:273:ILE:HD11	1.96	0.47
2:C:35:GLY:O	2:C:129:ASP:HB2	2.14	0.47
1:B:53:LYS:O	1:B:57:VAL:HG13	2.16	0.45
1:A:62:LEU:HD22	1:A:282:LEU:HD11	1.98	0.45
1:B:38:ILE:HD12	1:B:210:LYS:HB2	1.97	0.45
1:B:220:ILE:HD12	1:B:293:THR:HG21	1.99	0.45
1:A:240:LYS:HE3	8:D:1004:HOH:O	2.17	0.44
2:D:118:GLU:O	2:D:123:ALA:HB2	2.18	0.44
2:D:46:GLY:HA3	7:D:1000:ATP:O2'	2.18	0.44
2:C:102:LYS:HD2	7:C:1000:ATP:N7	2.33	0.43
7:D:1000:ATP:H5'2	8:D:1012:HOH:O	2.17	0.43
7:C:1000:ATP:H5'2	8:C:1005:HOH:O	2.19	0.43
1:B:74:HIS:CE1	1:B:117:ASN:HD22	2.15	0.43
1:A:74:HIS:HD2	1:A:75:GLY:O	2.01	0.43
1:B:59:ASP:OD2	1:B:279:HIS:HA	2.19	0.42
1:A:234:ILE:O	1:A:295:ILE:HA	2.20	0.42
2:D:49:ALA:HB2	2:D:64:GLU:HA	2.02	0.41
2:D:20:ARG:HA	2:D:21:PRO:HD3	1.94	0.41
1:A:284:GLU:O	4:A:1000:ARG:HB3	2.21	0.41
2:D:41:VAL:HA	2:D:72:LYS:O	2.21	0.40
1:B:284:GLU:HA	1:B:290:GLY:HA2	2.03	0.40
1:A:226:ASP:HA	1:A:227:PRO:HD3	1.77	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:115:ARG:NH1	7:C:1000:ATP:O1G[9_555]	2.19	0.01

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	279/298 (94%)	274 (98%)	4 (1%)	1 (0%)	39	61
1	B	281/298 (94%)	275 (98%)	5 (2%)	1 (0%)	39	61
2	C	123/135 (91%)	117 (95%)	5 (4%)	1 (1%)	24	41
2	D	124/135 (92%)	118 (95%)	4 (3%)	2 (2%)	12	21
All	All	807/866 (93%)	784 (97%)	18 (2%)	5 (1%)	30	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	51	GLY
1	A	76	GLY
1	B	76	GLY
2	D	64	GLU
2	D	128	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	225/239 (94%)	214 (95%)	11 (5%)	31	55
1	B	227/239 (95%)	217 (96%)	10 (4%)	35	60
2	C	104/114 (91%)	103 (99%)	1 (1%)	82	95
2	D	105/114 (92%)	103 (98%)	2 (2%)	65	87
All	All	661/706 (94%)	637 (96%)	24 (4%)	42	69

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	34	ARG
1	A	58	SER
1	A	66	VAL
1	A	88	ASN
1	A	147	VAL
1	A	161	ARG
1	A	168	ARG
1	A	230	LEU
1	A	263	LEU
1	A	282	LEU
1	B	23	LEU
1	B	27	LEU
1	B	49	SER
1	B	66	VAL
1	B	72	LEU
1	B	123	LEU
1	B	145	ARG
1	B	168	ARG
1	B	230	LEU
1	B	263	LEU
2	C	31	LEU
2	D	32	LEU
2	D	80	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	119	ASN
1	A	278	GLN
1	A	279	HIS
1	B	74	HIS
1	B	152	GLN
1	B	279	HIS
2	C	81	GLN
2	C	87	ASN
2	D	87	ASN

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 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	ARG	A	1000	-	5,11,11	0.35	0	3,13,13	0.66	0
5	ADP	A	2000	-	22,29,29	1.07	1 (4%)	27,45,45	1.77	3 (11%)
6	NLG	A	2001	-	6,12,12	4.86	2 (33%)	5,15,15	0.65	0
4	ARG	B	1000	-	5,11,11	0.37	0	3,13,13	0.81	0
5	ADP	B	2000	3	22,29,29	1.06	2 (9%)	27,45,45	1.84	3 (11%)
6	NLG	B	2001	-	6,12,12	4.68	2 (33%)	5,15,15	1.09	0
7	ATP	C	1000	3	24,33,33	1.18	2 (8%)	31,52,52	1.93	6 (19%)
7	ATP	D	1000	3	24,33,33	1.05	2 (8%)	31,52,52	1.90	7 (22%)

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
4	ARG	A	1000	-	-	0/5/11/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	A	2000	-	-	0/12/32/32	0/3/3/3
6	NLG	A	2001	-	-	0/7/13/13	0/0/0/0
4	ARG	B	1000	-	-	0/5/11/11	0/0/0/0
5	ADP	B	2000	3	-	0/12/32/32	0/3/3/3
6	NLG	B	2001	-	-	0/7/13/13	0/0/0/0
7	ATP	C	1000	3	-	0/18/38/38	0/3/3/3
7	ATP	D	1000	3	-	0/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2001	NLG	C8-C7	-9.11	1.32	1.50
6	B	2001	NLG	C8-C7	-8.77	1.32	1.50
6	A	2001	NLG	CA-N2	-7.65	1.35	1.46
6	B	2001	NLG	CA-N2	-7.39	1.35	1.46
5	B	2000	ADP	O4'-C1'	2.22	1.44	1.41
7	D	1000	ATP	O4'-C1'	2.40	1.44	1.41
7	D	1000	ATP	C5-C4	3.09	1.47	1.40
5	B	2000	ADP	C5-C4	3.21	1.47	1.40
7	C	1000	ATP	C5-C4	3.26	1.47	1.40
7	C	1000	ATP	O4'-C1'	3.34	1.45	1.41
5	A	2000	ADP	C5-C4	3.36	1.48	1.40

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	2000	ADP	N3-C2-N1	-7.54	123.12	128.89
5	A	2000	ADP	N3-C2-N1	-6.99	123.54	128.89
7	C	1000	ATP	N3-C2-N1	-6.86	123.64	128.89
7	D	1000	ATP	N3-C2-N1	-6.72	123.75	128.89
7	C	1000	ATP	PA-O3A-PB	-4.19	120.97	132.73
7	D	1000	ATP	PA-O3A-PB	-3.61	122.60	132.73
5	A	2000	ADP	C4-C5-N7	-2.92	106.80	109.48
7	D	1000	ATP	C4-C5-N7	-2.84	106.87	109.48
7	D	1000	ATP	C2'-C1'-N9	-2.80	110.01	114.29
7	C	1000	ATP	C4-C5-N7	-2.66	107.03	109.48
5	A	2000	ADP	PA-O3A-PB	-2.65	123.77	132.67
5	B	2000	ADP	C4-C5-N7	-2.65	107.04	109.48
7	D	1000	ATP	PB-O3B-PG	-2.63	123.86	132.67
5	B	2000	ADP	PA-O3A-PB	-2.34	124.84	132.67
7	C	1000	ATP	PB-O3B-PG	-2.08	125.70	132.67
7	D	1000	ATP	O4'-C4'-C5'	2.22	117.26	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	1000	ATP	O5'-C5'-C4'	2.35	117.77	109.12
7	C	1000	ATP	O4'-C4'-C5'	2.44	118.03	109.32
7	C	1000	ATP	O5'-C5'-C4'	3.16	120.76	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1000	ARG	2	0
7	C	1000	ATP	4	1
7	D	1000	ATP	5	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^{th} 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^2)	Q<0.9
1	A	281/298 (94%)	0.38	17 (6%) 25 28	52, 64, 93, 110	0
1	B	283/298 (94%)	0.54	26 (9%) 11 12	54, 63, 84, 115	0
2	C	125/135 (92%)	0.61	16 (12%) 5 5	55, 62, 80, 104	0
2	D	126/135 (93%)	0.65	14 (11%) 7 7	56, 65, 84, 124	0
All	All	815/866 (94%)	0.51	73 (8%) 12 12	52, 64, 90, 124	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	128	GLY	9.0
2	C	7	ILE	8.5
1	B	18	TYR	8.2
2	D	130	MET	7.7
1	A	225	GLU	7.3
2	D	7	ILE	5.9
1	B	15	SER	5.6
2	D	128	GLY	5.6
2	C	129	ASP	5.5
1	B	151	ALA	5.3
2	C	127	THR	5.2
2	C	52	GLY	5.0
1	B	16	PRO	4.8
1	A	18	TYR	4.7
1	A	297	GLY	4.5
2	D	14	LYS	4.4
2	D	129	ASP	4.3
2	D	106	LEU	4.2
1	A	241	LYS	4.1
1	A	223	ASN	3.9
2	D	127	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	247	LYS	3.8
1	B	179	ILE	3.5
1	B	73	VAL	3.4
2	C	106	LEU	3.2
1	B	178	VAL	3.2
1	B	150	SER	3.2
1	B	22	ILE	3.1
1	B	199	ALA	3.0
2	D	5	ASP	3.0
1	B	75	GLY	3.0
1	A	73	VAL	3.0
1	B	180	ALA	2.9
2	C	15	VAL	2.9
1	A	228	SER	2.9
1	B	148	PRO	2.8
2	C	14	LYS	2.8
1	B	17	ASP	2.8
2	C	16	GLU	2.7
1	A	245	ASP	2.7
2	C	104	PHE	2.6
1	A	186	ASP	2.6
1	B	40	VAL	2.5
1	A	244	GLU	2.5
1	A	113	VAL	2.5
1	A	224	LYS	2.5
1	B	228	SER	2.5
2	C	51	GLY	2.5
1	B	72	LEU	2.4
1	B	41	LYS	2.4
1	B	198	VAL	2.4
1	A	226	ASP	2.4
2	D	122	LYS	2.4
1	A	230	LEU	2.3
2	D	15	VAL	2.3
2	D	76	VAL	2.3
1	A	17	ASP	2.3
1	B	200	GLY	2.3
2	D	17	ALA	2.3
2	C	125	LYS	2.3
1	B	25	GLU	2.2
2	D	105	VAL	2.2
1	B	133	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	213	LEU	2.2
1	B	43	GLY	2.1
1	B	21	GLU	2.1
1	B	152	GLN	2.1
2	D	72	LYS	2.1
1	A	179	ILE	2.1
2	C	74	GLU	2.1
2	C	5	ASP	2.1
2	C	8	PRO	2.0
2	C	17	ALA	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^{th} 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^2)	Q<0.9
5	ADP	A	2000	27/27	0.53	0.38	1.86	71,75,95,98	27
3	MG	B	2002	1/1	0.73	0.33	1.30	65,65,65,65	0
4	ARG	A	1000	12/12	0.90	0.18	0.63	73,77,80,85	0
4	ARG	B	1000	12/12	0.87	0.20	0.56	68,73,74,76	0
6	NLG	A	2001	13/13	0.91	0.17	0.01	53,58,64,71	0
6	NLG	B	2001	13/13	0.92	0.13	-0.92	41,51,55,55	0
5	ADP	B	2000	27/27	0.96	0.12	-0.94	42,51,55,63	0
7	ATP	C	1000	31/31	0.94	0.12	-0.99	43,50,64,73	0
7	ATP	D	1000	31/31	0.95	0.12	-1.15	55,60,66,78	0
3	MG	C	1001	1/1	0.19	0.20	-	60,60,60,60	0
3	MG	D	1001	1/1	0.35	0.20	-	64,64,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.