



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:00 PM GMT

PDB ID : 4K8K  
Title : Crystal structure of probable sugar kinase protein from Rhizobium etli CFN 42 complexed with 1-(4-methoxyphenyl)-1-cyclopropane and 2-aminoperimidine  
Authors : Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth, S.; Kar, A.; Chan, M.K.; Laffuer, J.; Patel, H.; Matikainen, B.; Chamala, S.; Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Love, J.; Fiser, A.; Khafizov, K.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)  
Deposited on : 2013-04-18  
Resolution : 1.50 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

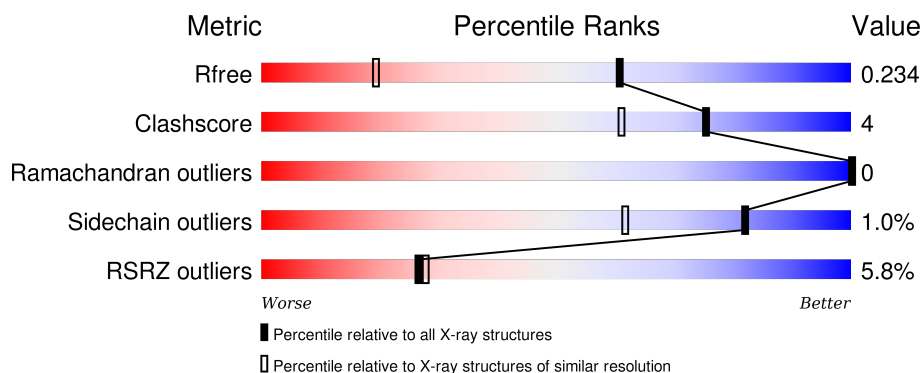
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


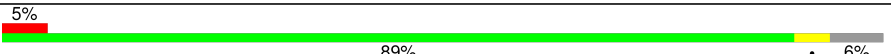
The reported resolution of this entry is 1.50 Å.

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))
$R_{free}$	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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	352	
1	B	352	

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
4	1PK	A	403	-	-	-	X
4	1PK	B	405	-	-	-	X
5	K	A	407	-	-	-	X
5	K	B	407	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6042 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 sugar kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	Se	0	10	0
			2571	1611	448	494	8	10			
1	B	330	Total	C	N	O	S	Se	0	8	0
			2545	1593	444	490	8	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MSE	-	EXPRESSION TAG	UNP Q2KDX6
A	-22	HIS	-	EXPRESSION TAG	UNP Q2KDX6
A	-21	HIS	-	EXPRESSION TAG	UNP Q2KDX6
A	-20	HIS	-	EXPRESSION TAG	UNP Q2KDX6
A	-19	HIS	-	EXPRESSION TAG	UNP Q2KDX6
A	-18	HIS	-	EXPRESSION TAG	UNP Q2KDX6
A	-17	HIS	-	EXPRESSION TAG	UNP Q2KDX6
A	-16	SER	-	EXPRESSION TAG	UNP Q2KDX6
A	-15	SER	-	EXPRESSION TAG	UNP Q2KDX6
A	-14	GLY	-	EXPRESSION TAG	UNP Q2KDX6
A	-13	VAL	-	EXPRESSION TAG	UNP Q2KDX6
A	-12	ASP	-	EXPRESSION TAG	UNP Q2KDX6
A	-11	LEU	-	EXPRESSION TAG	UNP Q2KDX6
A	-10	GLY	-	EXPRESSION TAG	UNP Q2KDX6
A	-9	THR	-	EXPRESSION TAG	UNP Q2KDX6
A	-8	GLU	-	EXPRESSION TAG	UNP Q2KDX6
A	-7	ASN	-	EXPRESSION TAG	UNP Q2KDX6
A	-6	LEU	-	EXPRESSION TAG	UNP Q2KDX6
A	-5	TYR	-	EXPRESSION TAG	UNP Q2KDX6
A	-4	PHE	-	EXPRESSION TAG	UNP Q2KDX6
A	-3	GLN	-	EXPRESSION TAG	UNP Q2KDX6
A	-2	SER	-	EXPRESSION TAG	UNP Q2KDX6
B	-23	MSE	-	EXPRESSION TAG	UNP Q2KDX6
B	-22	HIS	-	EXPRESSION TAG	UNP Q2KDX6
B	-21	HIS	-	EXPRESSION TAG	UNP Q2KDX6

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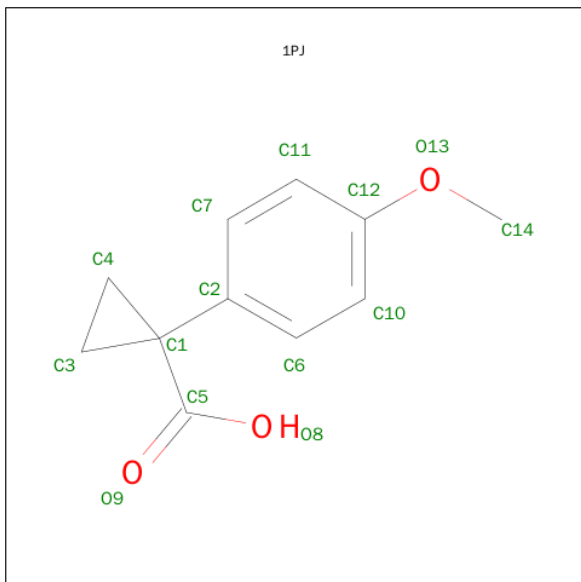
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	EXPRESSION TAG	UNP Q2KDX6
B	-19	HIS	-	EXPRESSION TAG	UNP Q2KDX6
B	-18	HIS	-	EXPRESSION TAG	UNP Q2KDX6
B	-17	HIS	-	EXPRESSION TAG	UNP Q2KDX6
B	-16	SER	-	EXPRESSION TAG	UNP Q2KDX6
B	-15	SER	-	EXPRESSION TAG	UNP Q2KDX6
B	-14	GLY	-	EXPRESSION TAG	UNP Q2KDX6
B	-13	VAL	-	EXPRESSION TAG	UNP Q2KDX6
B	-12	ASP	-	EXPRESSION TAG	UNP Q2KDX6
B	-11	LEU	-	EXPRESSION TAG	UNP Q2KDX6
B	-10	GLY	-	EXPRESSION TAG	UNP Q2KDX6
B	-9	THR	-	EXPRESSION TAG	UNP Q2KDX6
B	-8	GLU	-	EXPRESSION TAG	UNP Q2KDX6
B	-7	ASN	-	EXPRESSION TAG	UNP Q2KDX6
B	-6	LEU	-	EXPRESSION TAG	UNP Q2KDX6
B	-5	TYR	-	EXPRESSION TAG	UNP Q2KDX6
B	-4	PHE	-	EXPRESSION TAG	UNP Q2KDX6
B	-3	GLN	-	EXPRESSION TAG	UNP Q2KDX6
B	-2	SER	-	EXPRESSION TAG	UNP Q2KDX6

- Molecule 2 is ADENOSINE (three-letter code: ADN) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>4</sub>).



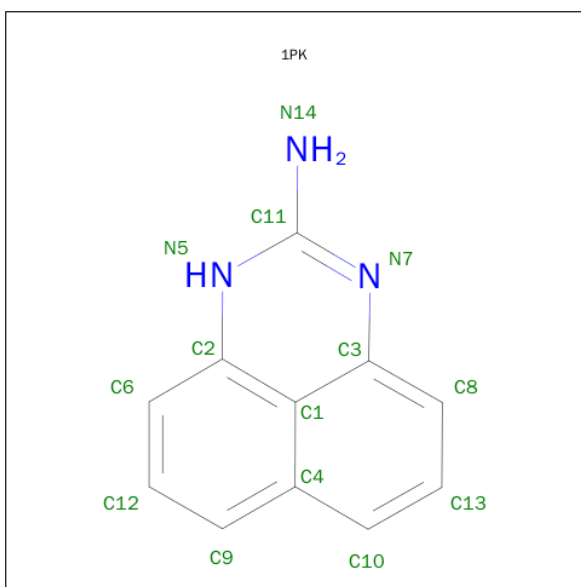
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	5	4		
2	B	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 3 is 1-(4-METHOXYPHENYL)CYCLOPROPANECARBOXYLIC ACID (three-letter code: 1PJ) (formula: C<sub>11</sub>H<sub>12</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	11	3		
3	B	1	Total	C	O	0	0
			14	11	3		

- Molecule 4 is 1H-PERIMIDIN-2-AMINE (three-letter code: 1PK) (formula: C<sub>11</sub>H<sub>9</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			14	11	3		
4	A	1	Total	C	N	0	0
			14	11	3		
4	A	1	Total	C	N	0	0
			14	11	3		
4	A	1	Total	C	N	0	0
			14	11	3		
4	B	1	Total	C	N	0	0
			14	11	3		
4	B	1	Total	C	N	0	0
			14	11	3		
4	B	1	Total	C	N	0	0
			14	11	3		
4	B	1	Total	C	N	0	0
			14	11	3		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	K	0	0
			1	1		
5	A	1	Total	K	0	0
			1	1		

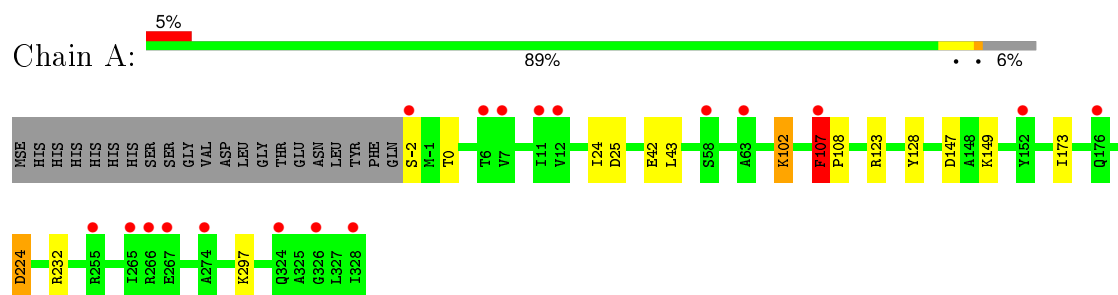
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	363	Total	O	0	0
			363	363		
6	B	383	Total	O	0	0
			383	383		

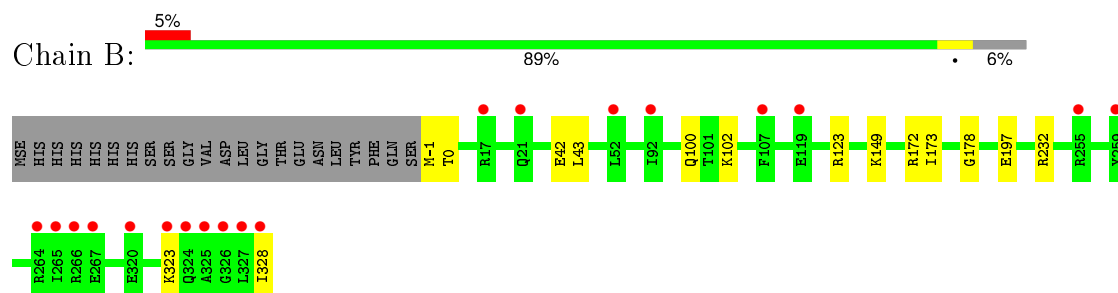
### 3 Residue-property plots [i](#)

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: sugar kinase



- Molecule 1: sugar kinase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.59Å 91.10Å 93.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.65 – 1.50 39.65 – 1.49	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.65-1.50) 99.5 (39.65-1.49)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 1.49Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.181 , 0.218 0.197 , 0.234	Depositor DCC
$R_{free}$ test set	5505 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.1	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	8 of 111808 reflections (0.007%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.48 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.3527e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 1PJ, 1PK, K, ADN

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	0.49	2/2629 (0.1%)	0.68	0/3536
1	B	0.50	0/2596	0.65	0/3493
All	All	0.49	2/5225 (0.0%)	0.66	0/7029

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107[A]	PHE	CA-C	5.63	1.67	1.52
1	A	107[B]	PHE	CA-C	5.63	1.67	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107[A]	PHE	Mainchain
1	A	107[B]	PHE	Mainchain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2571	0	2553	26	0
1	B	2545	0	2530	14	0
2	A	19	0	13	0	0
2	B	19	0	13	0	0
3	A	14	0	11	1	0
3	B	14	0	11	1	0
4	A	56	0	36	2	0
4	B	56	0	36	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	363	0	0	12	0
6	B	383	0	0	7	0
All	All	6042	0	5203	41	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 4.

All (41) 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:100:GLN:O	1:B:102:LYS:HE3	1.72	0.89
1:B:-1:MSE:O	6:B:702:HOH:O	2.02	0.77
1:A:102:LYS:HE3	6:A:744:HOH:O	1.87	0.74
1:A:102:LYS:CD	1:A:102:LYS:H	2.04	0.70
1:A:24:ILE:HG22	6:A:775:HOH:O	1.93	0.69
1:A:42:GLU:OE1	4:A:406:1PK:H9	1.92	0.69
1:A:25:ASP:HA	6:A:775:HOH:O	1.93	0.68
1:B:0:THR:HG21	1:B:149:LYS:HG3	1.77	0.64
1:A:0[B]:THR:HG21	1:A:149:LYS:HG3	1.79	0.64
1:A:0[A]:THR:HG23	6:A:629:HOH:O	1.99	0.62
1:A:224:ASP:HB3	6:A:832:HOH:O	2.00	0.62
1:A:102:LYS:HD3	1:A:102:LYS:N	2.15	0.61
1:B:178:GLY:HA2	6:B:876:HOH:O	1.99	0.61
1:A:102:LYS:H	1:A:102:LYS:CE	2.14	0.60
1:A:102:LYS:HD3	1:A:102:LYS:H	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:CD	1:A:102:LYS:N	2.66	0.59
1:B:197:GLU:HG3	6:B:681:HOH:O	2.02	0.58
1:A:0[B]:THR:HB	6:A:629:HOH:O	2.07	0.54
1:B:173:ILE:HD11	6:B:807:HOH:O	2.07	0.54
1:B:323:LYS:HG3	1:B:328:ILE:HG13	1.91	0.52
1:A:147:ASP:HB3	6:A:739:HOH:O	2.09	0.52
1:B:42:GLU:OE1	4:B:402:1PK:H9	2.11	0.50
1:A:297:LYS:NZ	6:A:841:HOH:O	2.37	0.50
1:B:-1:MSE:N	6:B:668:HOH:O	2.45	0.49
4:B:401:1PK:H9	3:B:404:1PJ:O9	2.12	0.49
1:A:173:ILE:HG12	6:A:772:HOH:O	2.13	0.48
1:B:172:ARG:NH2	6:B:814:HOH:O	2.47	0.47
1:A:232:ARG:NH2	6:A:663:HOH:O	2.47	0.47
1:B:42:GLU:HG2	4:B:401:1PK:N14	2.30	0.47
1:B:43:LEU:C	1:B:43:LEU:HD13	2.34	0.46
1:A:107[B]:PHE:CD2	1:A:108:PRO:HA	2.51	0.45
1:B:232:ARG:NH2	6:B:593:HOH:O	2.46	0.45
1:A:42:GLU:HG2	4:A:405:1PK:N14	2.30	0.45
1:A:107[A]:PHE:HA	1:A:108:PRO:C	2.37	0.45
1:A:24:ILE:C	6:A:775:HOH:O	2.55	0.45
1:A:0[A]:THR:CG2	6:A:629:HOH:O	2.61	0.44
1:A:128:TYR:CD2	3:A:402:1PJ:H12	2.54	0.43
1:A:102:LYS:HB2	1:A:102:LYS:HE2	1.92	0.42
1:B:0:THR:CG2	1:B:149:LYS:HE3	2.50	0.42
1:A:43:LEU:HD13	1:A:43:LEU:C	2.40	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	339/352 (96%)	333 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	336/352 (96%)	332 (99%)	4 (1%)	0	100	100
All	All	675/704 (96%)	665 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	268/266 (101%)	263 (98%)	5 (2%)	65	31
1	B	265/266 (100%)	263 (99%)	2 (1%)	86	70
All	All	533/532 (100%)	526 (99%)	7 (1%)	82	50

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	SER
1	A	102	LYS
1	A	123[A]	ARG
1	A	123[B]	ARG
1	A	224	ASP
1	B	123[A]	ARG
1	B	123[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	$\# Z  > 2$
2	ADN	A	401	-	16,21,21	1.07	1 (6%)	16,31,31	2.42	4 (25%)
3	1PJ	A	402	-	13,15,15	1.17	1 (7%)	16,22,22	1.43	3 (18%)
4	1PK	A	403	-	16,16,16	1.01	0	21,23,23	1.35	2 (9%)
4	1PK	A	404	-	16,16,16	1.14	0	21,23,23	1.41	2 (9%)
4	1PK	A	405	-	16,16,16	1.15	0	21,23,23	1.25	2 (9%)
4	1PK	A	406	-	16,16,16	1.14	0	21,23,23	1.35	1 (4%)
4	1PK	B	401	-	16,16,16	1.15	0	21,23,23	1.32	2 (9%)
4	1PK	B	402	-	16,16,16	1.15	0	21,23,23	1.48	3 (14%)
2	ADN	B	403	-	16,21,21	0.97	1 (6%)	16,31,31	2.52	4 (25%)
3	1PJ	B	404	-	13,15,15	1.10	1 (7%)	16,22,22	1.25	1 (6%)
4	1PK	B	405	-	16,16,16	1.02	0	21,23,23	1.43	3 (14%)
4	1PK	B	406	-	16,16,16	1.14	0	21,23,23	1.35	2 (9%)

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
2	ADN	A	401	-	-	0/2/22/22	0/3/3/3
3	1PJ	A	402	-	-	0/8/18/18	0/1/2/2
4	1PK	A	403	-	-	0/0/0/0	0/3/3/3
4	1PK	A	404	-	-	0/0/0/0	0/3/3/3
4	1PK	A	405	-	-	0/0/0/0	0/3/3/3
4	1PK	A	406	-	-	0/0/0/0	0/3/3/3
4	1PK	B	401	-	-	0/0/0/0	0/3/3/3
4	1PK	B	402	-	-	0/0/0/0	0/3/3/3
2	ADN	B	403	-	-	0/2/22/22	0/3/3/3
3	1PJ	B	404	-	-	0/8/18/18	0/1/2/2
4	1PK	B	405	-	-	0/0/0/0	0/3/3/3
4	1PK	B	406	-	-	0/0/0/0	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	1PJ	C1-C2	-3.34	1.49	1.54
3	B	404	1PJ	C1-C2	-2.87	1.50	1.54
2	B	403	ADN	C5-C4	2.95	1.47	1.40
2	A	401	ADN	C5-C4	2.98	1.47	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	ADN	N3-C2-N1	-6.55	123.88	128.89
2	A	401	ADN	N3-C2-N1	-6.45	123.96	128.89
2	B	403	ADN	C4'-O4'-C1'	-5.23	103.97	109.72
2	A	401	ADN	C4'-O4'-C1'	-4.35	104.94	109.72
4	B	402	1PK	N5-C11-N7	-4.34	120.42	127.23
2	A	401	ADN	C1'-N9-C4	-4.27	120.49	126.94
4	A	404	1PK	N5-C11-N7	-4.15	120.71	127.23
4	B	405	1PK	N5-C11-N7	-4.15	120.71	127.23
4	B	406	1PK	N5-C11-N7	-4.11	120.77	127.23
4	A	406	1PK	N5-C11-N7	-4.03	120.90	127.23
2	B	403	ADN	C1'-N9-C4	-3.97	120.95	126.94
4	B	401	1PK	N5-C11-N7	-3.90	121.10	127.23
4	A	403	1PK	N5-C11-N7	-3.82	121.23	127.23
4	A	405	1PK	N5-C11-N7	-3.63	121.54	127.23
4	B	402	1PK	C1-C2-N5	-3.03	118.51	120.90
4	A	403	1PK	C1-C2-N5	-2.72	118.75	120.90
3	A	402	1PJ	C4-C1-C2	-2.65	114.73	119.86
4	A	404	1PK	C1-C2-N5	-2.54	118.90	120.90
4	B	405	1PK	C1-C2-N5	-2.30	119.08	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	405	1PK	C1-C3-N7	-2.26	119.11	120.90
4	A	405	1PK	C1-C2-N5	-2.25	119.12	120.90
4	B	401	1PK	C1-C3-N7	-2.13	119.22	120.90
4	B	406	1PK	C1-C3-N7	-2.09	119.25	120.90
3	A	402	1PJ	C7-C2-C6	2.14	121.15	117.94
4	B	402	1PK	C4-C1-C3	2.25	121.10	118.31
2	A	401	ADN	C2-N1-C6	2.47	123.17	118.77
2	B	403	ADN	C2-N1-C6	2.75	123.69	118.77
3	B	404	1PJ	C3-C1-C4	3.06	60.56	58.68
3	A	402	1PJ	C3-C1-C4	3.14	60.62	58.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	1PJ	1	0
4	A	405	1PK	1	0
4	A	406	1PK	1	0
4	B	401	1PK	2	0
4	B	402	1PK	1	0
3	B	404	1PJ	1	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	321/352 (91%)	0.37	18 (5%) 28 29	7, 11, 21, 38	0
1	B	320/352 (90%)	0.34	19 (5%) 26 27	6, 11, 21, 50	0
All	All	641/704 (91%)	0.35	37 (5%) 26 28	6, 11, 21, 50	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	264	ARG	6.7
1	A	-2	SER	5.8
1	B	324	GLN	4.9
1	A	328	ILE	4.9
1	B	266	ARG	4.7
1	B	255	ARG	4.2
1	A	266	ARG	4.1
1	B	92[A]	ILE	3.5
1	B	326	GLY	3.5
1	B	267	GLU	3.3
1	A	265	ILE	3.2
1	B	259	TYR	3.2
1	A	326	GLY	2.8
1	B	265	ILE	2.7
1	A	324	GLN	2.6
1	A	7	VAL	2.6
1	B	119	GLU	2.5
1	A	176	GLN	2.5
1	B	52	LEU	2.3
1	A	152	TYR	2.3
1	A	11	ILE	2.3
1	A	255	ARG	2.2
1	B	17	ARG	2.2
1	A	267	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	21	GLN	2.1
1	A	6	THR	2.1
1	A	107[A]	PHE	2.1
1	A	12	VAL	2.1
1	B	107	PHE	2.1
1	B	327	LEU	2.1
1	A	63	ALA	2.0
1	A	274	ALA	2.0
1	A	58[A]	SER	2.0
1	B	328	ILE	2.0
1	B	320	GLU	2.0
1	B	325	ALA	2.0
1	B	323	LYS	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
4	1PK	B	405	14/14	0.84	0.21	7.70	11,14,18,19	0
5	K	B	407	1/1	0.99	0.15	6.64	31,31,31,31	0
4	1PK	A	403	14/14	0.89	0.19	2.78	10,11,13,13	0
5	K	A	407	1/1	0.99	0.13	2.49	31,31,31,31	0
3	1PJ	A	402	14/14	0.88	0.11	0.59	11,12,14,15	0
3	1PJ	B	404	14/14	0.89	0.09	0.59	10,11,13,13	0
2	ADN	B	403	19/19	0.96	0.11	0.06	6,7,8,9	0
2	ADN	A	401	19/19	0.95	0.12	-0.06	7,8,9,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	1PK	B	406	14/14	0.78	0.26	-	14,17,21,26	14
4	1PK	B	402	14/14	0.60	0.23	-	19,21,22,23	14
4	1PK	A	404	14/14	0.90	0.15	-	13,15,16,19	14
4	1PK	A	406	14/14	0.57	0.35	-	17,18,20,23	14
4	1PK	B	401	14/14	0.70	0.20	-	15,17,20,26	14
4	1PK	A	405	14/14	0.60	0.26	-	16,17,20,23	14

## 6.5 Other polymers [i](#)

There are no such residues in this entry.