



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 05:25 am BST

PDB ID : 5V6D  
Title : Crystal structure of nucleoside diphosphate kinase from *Neisseria gonorrhoeae* in complex with citrate  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2017-03-16  
Resolution : 1.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

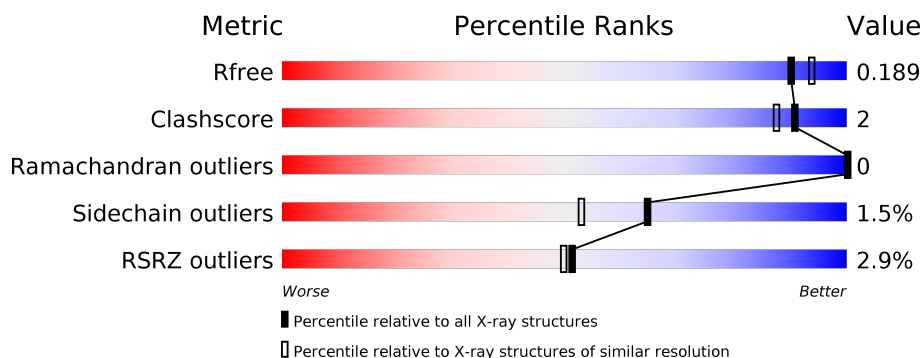
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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))
$R_{free}$	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 respectively. 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	149	<div> <div>9%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>
1	B	149	<div> <div>%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
1	C	149	<div> <div>%</div> <div>89%</div> <div>5%</div> <div>7%</div> </div>
1	D	149	<div> <div>%</div> <div>91%</div> <div>•</div> <div>6%</div> </div>
1	E	149	<div> <div>%</div> <div>89%</div> <div>•</div> <div>7%</div> </div>
1	F	149	<div> <div>%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	149	
1	H	149	
1	I	149	
1	J	149	
1	K	149	
1	L	149	
1	M	149	
1	N	149	
1	O	149	
1	P	149	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20042 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	4	0
			1083	683	185	210	5			
1	B	140	Total	C	N	O	S	0	4	0
			1081	686	180	210	5			
1	C	139	Total	C	N	O	S	0	4	0
			1083	690	183	204	6			
1	D	140	Total	C	N	O	S	0	6	0
			1090	695	187	203	5			
1	E	139	Total	C	N	O	S	0	9	0
			1104	707	184	208	5			
1	F	141	Total	C	N	O	S	0	5	0
			1095	699	183	208	5			
1	G	141	Total	C	N	O	S	0	6	0
			1104	704	186	208	6			
1	H	141	Total	C	N	O	S	0	9	0
			1117	712	189	211	5			
1	I	140	Total	C	N	O	S	0	7	0
			1110	703	189	213	5			
1	J	141	Total	C	N	O	S	0	2	0
			1085	690	183	207	5			
1	K	140	Total	C	N	O	S	0	7	0
			1096	701	181	208	6			
1	L	141	Total	C	N	O	S	0	11	0
			1132	729	185	212	6			
1	M	141	Total	C	N	O	S	0	4	0
			1095	697	183	210	5			
1	N	141	Total	C	N	O	S	0	3	0
			1084	690	182	207	5			
1	O	139	Total	C	N	O	S	0	4	0
			1066	678	180	202	6			
1	P	141	Total	C	N	O	S	0	3	0
			1077	686	180	205	6			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP B4RMG0
A	-6	ALA	-	expression tag	UNP B4RMG0
A	-5	HIS	-	expression tag	UNP B4RMG0
A	-4	HIS	-	expression tag	UNP B4RMG0
A	-3	HIS	-	expression tag	UNP B4RMG0
A	-2	HIS	-	expression tag	UNP B4RMG0
A	-1	HIS	-	expression tag	UNP B4RMG0
A	0	HIS	-	expression tag	UNP B4RMG0
B	-7	MET	-	expression tag	UNP B4RMG0
B	-6	ALA	-	expression tag	UNP B4RMG0
B	-5	HIS	-	expression tag	UNP B4RMG0
B	-4	HIS	-	expression tag	UNP B4RMG0
B	-3	HIS	-	expression tag	UNP B4RMG0
B	-2	HIS	-	expression tag	UNP B4RMG0
B	-1	HIS	-	expression tag	UNP B4RMG0
B	0	HIS	-	expression tag	UNP B4RMG0
C	-7	MET	-	expression tag	UNP B4RMG0
C	-6	ALA	-	expression tag	UNP B4RMG0
C	-5	HIS	-	expression tag	UNP B4RMG0
C	-4	HIS	-	expression tag	UNP B4RMG0
C	-3	HIS	-	expression tag	UNP B4RMG0
C	-2	HIS	-	expression tag	UNP B4RMG0
C	-1	HIS	-	expression tag	UNP B4RMG0
C	0	HIS	-	expression tag	UNP B4RMG0
D	-7	MET	-	expression tag	UNP B4RMG0
D	-6	ALA	-	expression tag	UNP B4RMG0
D	-5	HIS	-	expression tag	UNP B4RMG0
D	-4	HIS	-	expression tag	UNP B4RMG0
D	-3	HIS	-	expression tag	UNP B4RMG0
D	-2	HIS	-	expression tag	UNP B4RMG0
D	-1	HIS	-	expression tag	UNP B4RMG0
D	0	HIS	-	expression tag	UNP B4RMG0
E	-7	MET	-	expression tag	UNP B4RMG0
E	-6	ALA	-	expression tag	UNP B4RMG0
E	-5	HIS	-	expression tag	UNP B4RMG0
E	-4	HIS	-	expression tag	UNP B4RMG0
E	-3	HIS	-	expression tag	UNP B4RMG0
E	-2	HIS	-	expression tag	UNP B4RMG0
E	-1	HIS	-	expression tag	UNP B4RMG0
E	0	HIS	-	expression tag	UNP B4RMG0
F	-7	MET	-	expression tag	UNP B4RMG0
F	-6	ALA	-	expression tag	UNP B4RMG0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	HIS	-	expression tag	UNP B4RMG0
F	-4	HIS	-	expression tag	UNP B4RMG0
F	-3	HIS	-	expression tag	UNP B4RMG0
F	-2	HIS	-	expression tag	UNP B4RMG0
F	-1	HIS	-	expression tag	UNP B4RMG0
F	0	HIS	-	expression tag	UNP B4RMG0
G	-7	MET	-	expression tag	UNP B4RMG0
G	-6	ALA	-	expression tag	UNP B4RMG0
G	-5	HIS	-	expression tag	UNP B4RMG0
G	-4	HIS	-	expression tag	UNP B4RMG0
G	-3	HIS	-	expression tag	UNP B4RMG0
G	-2	HIS	-	expression tag	UNP B4RMG0
G	-1	HIS	-	expression tag	UNP B4RMG0
G	0	HIS	-	expression tag	UNP B4RMG0
H	-7	MET	-	expression tag	UNP B4RMG0
H	-6	ALA	-	expression tag	UNP B4RMG0
H	-5	HIS	-	expression tag	UNP B4RMG0
H	-4	HIS	-	expression tag	UNP B4RMG0
H	-3	HIS	-	expression tag	UNP B4RMG0
H	-2	HIS	-	expression tag	UNP B4RMG0
H	-1	HIS	-	expression tag	UNP B4RMG0
H	0	HIS	-	expression tag	UNP B4RMG0
I	-7	MET	-	expression tag	UNP B4RMG0
I	-6	ALA	-	expression tag	UNP B4RMG0
I	-5	HIS	-	expression tag	UNP B4RMG0
I	-4	HIS	-	expression tag	UNP B4RMG0
I	-3	HIS	-	expression tag	UNP B4RMG0
I	-2	HIS	-	expression tag	UNP B4RMG0
I	-1	HIS	-	expression tag	UNP B4RMG0
I	0	HIS	-	expression tag	UNP B4RMG0
J	-7	MET	-	expression tag	UNP B4RMG0
J	-6	ALA	-	expression tag	UNP B4RMG0
J	-5	HIS	-	expression tag	UNP B4RMG0
J	-4	HIS	-	expression tag	UNP B4RMG0
J	-3	HIS	-	expression tag	UNP B4RMG0
J	-2	HIS	-	expression tag	UNP B4RMG0
J	-1	HIS	-	expression tag	UNP B4RMG0
J	0	HIS	-	expression tag	UNP B4RMG0
K	-7	MET	-	expression tag	UNP B4RMG0
K	-6	ALA	-	expression tag	UNP B4RMG0
K	-5	HIS	-	expression tag	UNP B4RMG0
K	-4	HIS	-	expression tag	UNP B4RMG0

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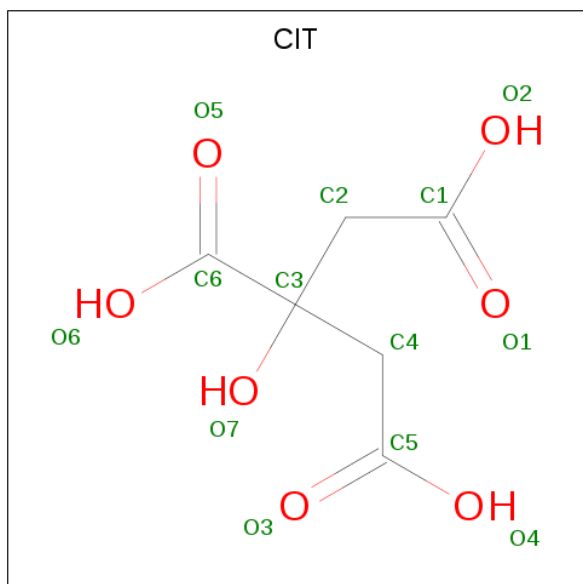
Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	HIS	-	expression tag	UNP B4RMG0
K	-2	HIS	-	expression tag	UNP B4RMG0
K	-1	HIS	-	expression tag	UNP B4RMG0
K	0	HIS	-	expression tag	UNP B4RMG0
L	-7	MET	-	expression tag	UNP B4RMG0
L	-6	ALA	-	expression tag	UNP B4RMG0
L	-5	HIS	-	expression tag	UNP B4RMG0
L	-4	HIS	-	expression tag	UNP B4RMG0
L	-3	HIS	-	expression tag	UNP B4RMG0
L	-2	HIS	-	expression tag	UNP B4RMG0
L	-1	HIS	-	expression tag	UNP B4RMG0
L	0	HIS	-	expression tag	UNP B4RMG0
M	-7	MET	-	expression tag	UNP B4RMG0
M	-6	ALA	-	expression tag	UNP B4RMG0
M	-5	HIS	-	expression tag	UNP B4RMG0
M	-4	HIS	-	expression tag	UNP B4RMG0
M	-3	HIS	-	expression tag	UNP B4RMG0
M	-2	HIS	-	expression tag	UNP B4RMG0
M	-1	HIS	-	expression tag	UNP B4RMG0
M	0	HIS	-	expression tag	UNP B4RMG0
N	-7	MET	-	expression tag	UNP B4RMG0
N	-6	ALA	-	expression tag	UNP B4RMG0
N	-5	HIS	-	expression tag	UNP B4RMG0
N	-4	HIS	-	expression tag	UNP B4RMG0
N	-3	HIS	-	expression tag	UNP B4RMG0
N	-2	HIS	-	expression tag	UNP B4RMG0
N	-1	HIS	-	expression tag	UNP B4RMG0
N	0	HIS	-	expression tag	UNP B4RMG0
O	-7	MET	-	expression tag	UNP B4RMG0
O	-6	ALA	-	expression tag	UNP B4RMG0
O	-5	HIS	-	expression tag	UNP B4RMG0
O	-4	HIS	-	expression tag	UNP B4RMG0
O	-3	HIS	-	expression tag	UNP B4RMG0
O	-2	HIS	-	expression tag	UNP B4RMG0
O	-1	HIS	-	expression tag	UNP B4RMG0
O	0	HIS	-	expression tag	UNP B4RMG0
P	-7	MET	-	expression tag	UNP B4RMG0
P	-6	ALA	-	expression tag	UNP B4RMG0
P	-5	HIS	-	expression tag	UNP B4RMG0
P	-4	HIS	-	expression tag	UNP B4RMG0
P	-3	HIS	-	expression tag	UNP B4RMG0
P	-2	HIS	-	expression tag	UNP B4RMG0

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-1	HIS	-	expression tag	UNP B4RMG0
P	0	HIS	-	expression tag	UNP B4RMG0

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		
2	G	1	Total	C	O	0	0
			13	6	7		
2	H	1	Total	C	O	0	0
			13	6	7		
2	I	1	Total	C	O	0	0
			13	6	7		
2	J	1	Total	C	O	0	0
			13	6	7		

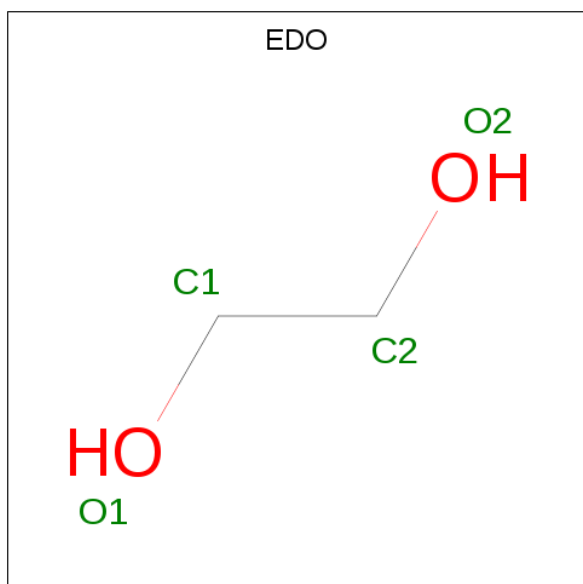
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	K	1	Total	C	O	0	0
			13	6	7		
2	L	1	Total	C	O	0	0
			13	6	7		
2	M	1	Total	C	O	0	0
			13	6	7		
2	N	1	Total	C	O	0	0
			13	6	7		
2	O	1	Total	C	O	0	0
			13	6	7		
2	P	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	K	1	Total C O 4 2 2	0	0
3	K	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	M	1	Total C O 4 2 2	0	0
3	M	1	Total C O 4 2 2	0	0
3	N	1	Total C O 4 2 2	0	0
3	O	1	Total C O 4 2 2	0	0
3	P	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	70	Total O 72 72	0	2
4	B	129	Total O 130 130	0	1

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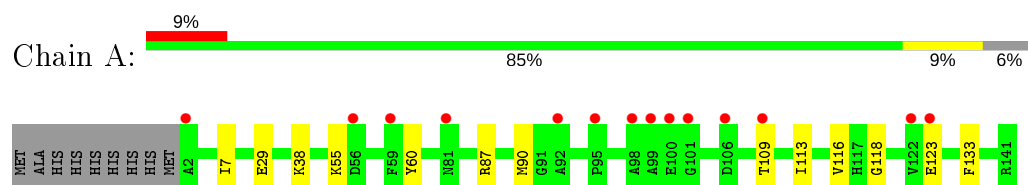
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	166	Total 166	O 166	0	0
4	D	139	Total 141	O 141	0	2
4	E	146	Total 148	O 148	0	2
4	F	174	Total 175	O 175	0	1
4	G	149	Total 151	O 151	0	2
4	H	155	Total 156	O 156	0	1
4	I	174	Total 177	O 177	0	3
4	J	156	Total 160	O 160	0	4
4	K	144	Total 146	O 146	0	2
4	L	159	Total 160	O 160	0	1
4	M	133	Total 134	O 134	0	1
4	N	129	Total 129	O 129	0	0
4	O	77	Total 77	O 77	0	0
4	P	119	Total 122	O 122	0	3

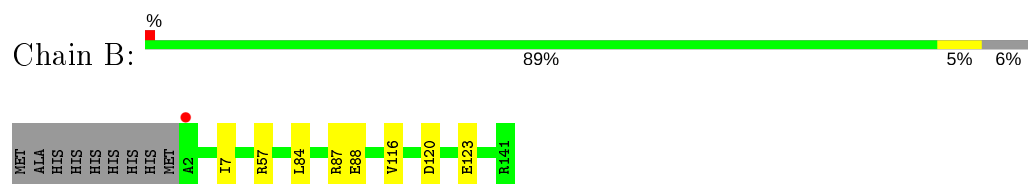
### 3 Residue-property plots [i](#)

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.

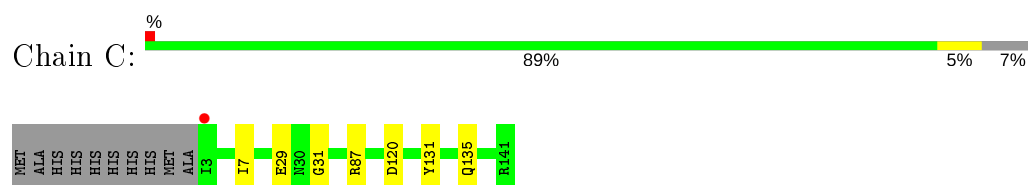
- Molecule 1: Nucleoside diphosphate kinase



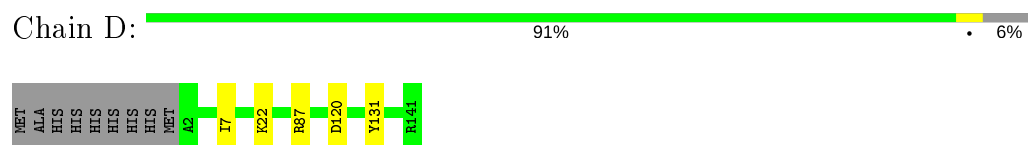
- Molecule 1: Nucleoside diphosphate kinase



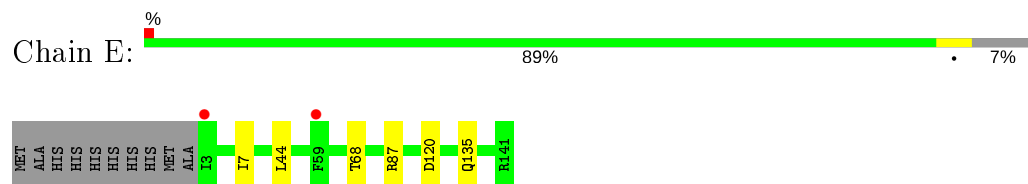
- Molecule 1: Nucleoside diphosphate kinase



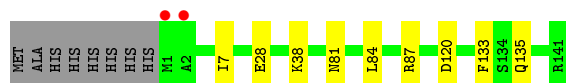
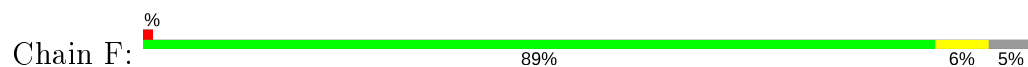
- Molecule 1: Nucleoside diphosphate kinase



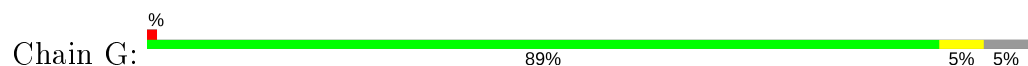
- Molecule 1: Nucleoside diphosphate kinase



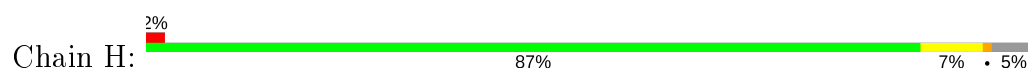
- Molecule 1: Nucleoside diphosphate kinase



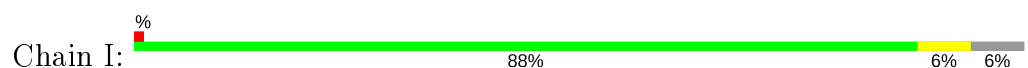
- Molecule 1: Nucleoside diphosphate kinase



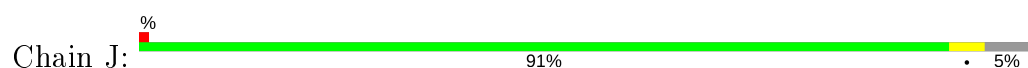
- Molecule 1: Nucleoside diphosphate kinase



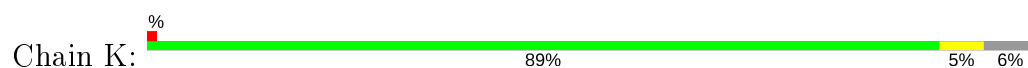
- Molecule 1: Nucleoside diphosphate kinase



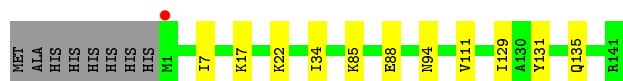
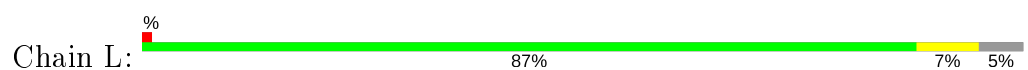
- Molecule 1: Nucleoside diphosphate kinase



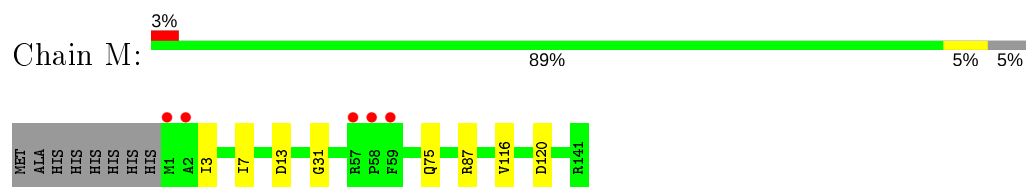
- Molecule 1: Nucleoside diphosphate kinase



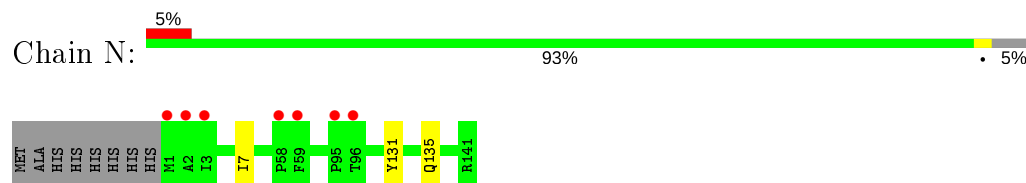
- Molecule 1: Nucleoside diphosphate kinase



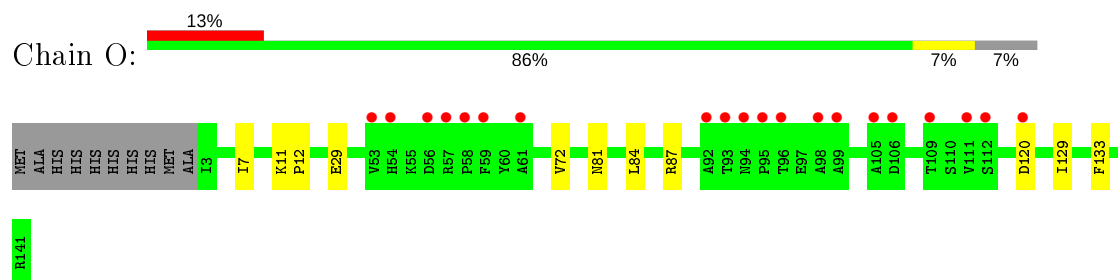
- Molecule 1: Nucleoside diphosphate kinase



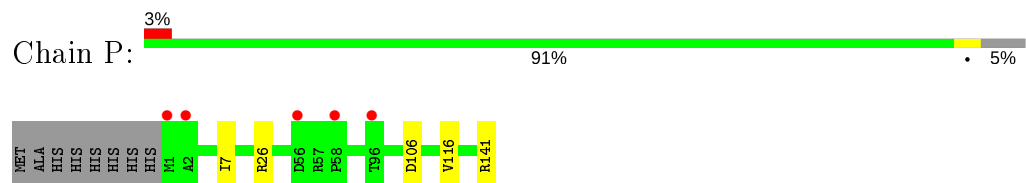
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.24Å 112.35Å 112.87Å 104.31° 98.50° 105.39°	Depositor
Resolution (Å)	44.09 – 1.85 44.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.1 (44.09-1.85) 97.1 (44.99-1.85)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 1.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.150 , 0.188 0.150 , 0.189	Depositor DCC
$R_{free}$ test set	1976 reflections (0.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	20042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CIT

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	0.27	0/1103	0.46	0/1491
1	B	0.34	0/1107	0.51	0/1497
1	C	0.35	0/1112	0.53	0/1499
1	D	0.33	0/1125	0.50	0/1521
1	E	0.33	0/1145	0.50	0/1545
1	F	0.36	0/1128	0.53	0/1524
1	G	0.35	0/1139	0.52	0/1537
1	H	0.32	0/1156	0.50	0/1561
1	I	0.35	0/1139	0.51	0/1537
1	J	0.35	0/1108	0.52	0/1495
1	K	0.35	0/1134	0.51	0/1531
1	L	0.36	0/1182	0.53	0/1594
1	M	0.33	0/1124	0.50	0/1518
1	N	0.33	0/1110	0.50	0/1501
1	O	0.29	0/1095	0.46	0/1480
1	P	0.33	0/1103	0.49	0/1492
All	All	0.33	0/18010	0.51	0/24323

There are no bond length outliers.

There are no bond angle outliers.

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	1083	0	1062	7	0
1	B	1081	0	1067	3	0
1	C	1083	0	1104	5	0
1	D	1090	0	1107	3	0
1	E	1104	0	1130	3	0
1	F	1095	0	1112	5	0
1	G	1104	0	1127	3	0
1	H	1117	0	1135	6	0
1	I	1110	0	1115	4	0
1	J	1085	0	1099	2	0
1	K	1096	0	1117	5	0
1	L	1132	0	1181	8	0
1	M	1095	0	1109	3	0
1	N	1084	0	1089	2	0
1	O	1066	0	1065	7	0
1	P	1077	0	1080	2	0
2	A	13	0	5	1	0
2	B	13	0	5	0	0
2	C	13	0	5	0	0
2	D	13	0	5	0	0
2	E	13	0	5	0	0
2	F	13	0	5	0	0
2	G	13	0	5	0	0
2	H	13	0	5	0	0
2	I	13	0	5	0	0
2	J	13	0	5	0	0
2	K	13	0	5	0	0
2	L	13	0	5	0	0
2	M	13	0	5	0	0
2	N	13	0	5	0	0
2	O	13	0	5	0	0
2	P	13	0	5	0	0
3	A	8	0	12	0	0
3	B	4	0	6	0	0
3	C	8	0	12	0	0
3	D	4	0	6	0	0
3	E	4	0	6	0	0
3	F	4	0	6	0	0
3	G	4	0	6	0	0
3	H	12	0	18	1	0
3	I	4	0	6	0	0
3	J	4	0	6	0	0
3	K	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	4	0	6	0	0
3	M	8	0	12	0	0
3	N	4	0	6	0	0
3	O	4	0	6	0	0
3	P	4	0	6	0	0
4	A	72	0	0	0	0
4	B	130	0	0	0	0
4	C	166	0	0	1	0
4	D	141	0	0	0	0
4	E	148	0	0	0	0
4	F	175	0	0	0	0
4	G	151	0	0	0	0
4	H	156	0	0	1	0
4	I	177	0	0	1	0
4	J	160	0	0	0	0
4	K	146	0	0	1	0
4	L	160	0	0	1	0
4	M	134	0	0	0	0
4	N	129	0	0	0	0
4	O	77	0	0	0	0
4	P	122	0	0	1	0
All	All	20042	0	17911	61	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 2.

The worst 5 of 61 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:O:81:ASN:HD21	1:O:84:LEU:HD23	1.51	0.75
1:F:81:ASN:HD21	1:F:84:LEU:HD23	1.53	0.72
1:C:135:GLN:NE2	4:C:301:HOH:O	2.24	0.69
1:G:26:ARG:NH2	1:G:106:ASP:OD2	2.25	0.65
1:P:26:ARG:NH2	1:P:106:ASP:OD2	2.29	0.64

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	142/149 (95%)	136 (96%)	6 (4%)	0	100	100
1	B	142/149 (95%)	140 (99%)	2 (1%)	0	100	100
1	C	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	D	144/149 (97%)	142 (99%)	2 (1%)	0	100	100
1	E	145/149 (97%)	143 (99%)	2 (1%)	0	100	100
1	F	144/149 (97%)	142 (99%)	2 (1%)	0	100	100
1	G	145/149 (97%)	143 (99%)	2 (1%)	0	100	100
1	H	148/149 (99%)	144 (97%)	4 (3%)	0	100	100
1	I	145/149 (97%)	141 (97%)	4 (3%)	0	100	100
1	J	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	K	145/149 (97%)	143 (99%)	2 (1%)	0	100	100
1	L	150/149 (101%)	148 (99%)	2 (1%)	0	100	100
1	M	143/149 (96%)	141 (99%)	2 (1%)	0	100	100
1	N	142/149 (95%)	140 (99%)	2 (1%)	0	100	100
1	O	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
1	P	142/149 (95%)	140 (99%)	2 (1%)	0	100	100
All	All	2300/2384 (96%)	2260 (98%)	40 (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	111/121 (92%)	109 (98%)	2 (2%)	59	45
1	B	112/121 (93%)	109 (97%)	3 (3%)	44	29
1	C	115/121 (95%)	114 (99%)	1 (1%)	78	72
1	D	114/121 (94%)	113 (99%)	1 (1%)	78	72
1	E	118/121 (98%)	117 (99%)	1 (1%)	81	76
1	F	116/121 (96%)	115 (99%)	1 (1%)	78	72
1	G	117/121 (97%)	115 (98%)	2 (2%)	60	47
1	H	118/121 (98%)	114 (97%)	4 (3%)	37	19
1	I	117/121 (97%)	115 (98%)	2 (2%)	60	47
1	J	114/121 (94%)	112 (98%)	2 (2%)	59	45
1	K	117/121 (97%)	116 (99%)	1 (1%)	78	72
1	L	123/121 (102%)	121 (98%)	2 (2%)	62	49
1	M	116/121 (96%)	111 (96%)	5 (4%)	29	12
1	N	113/121 (93%)	112 (99%)	1 (1%)	78	72
1	O	111/121 (92%)	111 (100%)	0	100	100
1	P	112/121 (93%)	110 (98%)	2 (2%)	59	45
All	All	1844/1936 (95%)	1814 (98%)	30 (2%)	65	49

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	93	THR
1	I	116	VAL
1	N	7	ILE
1	I	7	ILE
1	J	7	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	81	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 ⓘ

38 ligands are modelled in this entry.

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	CIT	P	201	-	3,12,12	1.35	0	3,17,17	2.11	2 (66%)
2	CIT	M	201	-	3,12,12	1.07	0	3,17,17	2.45	2 (66%)
2	CIT	N	201	-	3,12,12	1.39	0	3,17,17	2.59	2 (66%)
2	CIT	O	201	-	3,12,12	1.33	0	3,17,17	2.09	1 (33%)
2	CIT	J	201	-	3,12,12	1.65	0	3,17,17	2.60	2 (66%)
3	EDO	D	202	-	3,3,3	0.42	0	2,2,2	0.31	0
2	CIT	B	201	-	3,12,12	1.33	0	3,17,17	2.13	2 (66%)
2	CIT	C	201	-	3,12,12	1.56	0	3,17,17	2.76	2 (66%)
3	EDO	K	202	-	3,3,3	0.45	0	2,2,2	0.26	0
3	EDO	H	201	-	3,3,3	0.47	0	2,2,2	0.34	0
3	EDO	P	202	-	3,3,3	0.44	0	2,2,2	0.40	0
2	CIT	I	201	-	3,12,12	1.35	0	3,17,17	2.54	2 (66%)
3	EDO	C	203	-	3,3,3	0.47	0	2,2,2	0.39	0
3	EDO	C	202	-	3,3,3	0.48	0	2,2,2	0.31	0
2	CIT	G	201	-	3,12,12	1.28	0	3,17,17	2.44	2 (66%)
3	EDO	A	202	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	L	202	-	3,3,3	0.39	0	2,2,2	0.31	0
3	EDO	M	202	-	3,3,3	0.43	0	2,2,2	0.31	0
3	EDO	J	202	-	3,3,3	0.41	0	2,2,2	0.57	0
3	EDO	G	202	-	3,3,3	0.40	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	H	203	-	3,3,3	0.46	0	2,2,2	0.35	0
3	EDO	A	203	-	3,3,3	0.47	0	2,2,2	0.21	0
3	EDO	M	203	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EDO	K	203	-	3,3,3	0.50	0	2,2,2	0.38	0
2	CIT	L	201	-	3,12,12	1.54	0	3,17,17	2.48	1 (33%)
3	EDO	N	202	-	3,3,3	0.45	0	2,2,2	0.37	0
3	EDO	I	202	-	3,3,3	0.37	0	2,2,2	0.58	0
3	EDO	H	204	-	3,3,3	0.46	0	2,2,2	0.08	0
2	CIT	K	201	-	3,12,12	1.23	0	3,17,17	2.86	2 (66%)
2	CIT	E	201	-	3,12,12	1.76	0	3,17,17	3.08	2 (66%)
2	CIT	F	201	-	3,12,12	1.17	0	3,17,17	2.44	1 (33%)
3	EDO	F	202	-	3,3,3	0.41	0	2,2,2	0.40	0
3	EDO	E	202	-	3,3,3	0.45	0	2,2,2	0.33	0
2	CIT	A	201	-	3,12,12	1.38	0	3,17,17	2.40	2 (66%)
3	EDO	O	202	-	3,3,3	0.46	0	2,2,2	0.38	0
3	EDO	B	202	-	3,3,3	0.40	0	2,2,2	0.38	0
2	CIT	H	202	-	3,12,12	1.39	0	3,17,17	1.77	2 (66%)
2	CIT	D	201	-	3,12,12	1.69	0	3,17,17	3.02	2 (66%)

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	CIT	P	201	-	-	0/6/16/16	-
2	CIT	M	201	-	-	0/6/16/16	-
2	CIT	N	201	-	-	0/6/16/16	-
2	CIT	O	201	-	-	0/6/16/16	-
2	CIT	J	201	-	-	0/6/16/16	-
3	EDO	D	202	-	-	0/1/1/1	-
2	CIT	B	201	-	-	0/6/16/16	-
2	CIT	C	201	-	-	0/6/16/16	-
3	EDO	K	202	-	-	0/1/1/1	-
3	EDO	H	201	-	-	0/1/1/1	-
3	EDO	P	202	-	-	0/1/1/1	-
2	CIT	I	201	-	-	0/6/16/16	-
3	EDO	C	203	-	-	0/1/1/1	-
3	EDO	C	202	-	-	0/1/1/1	-
2	CIT	G	201	-	-	0/6/16/16	-
3	EDO	A	202	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	L	202	-	-	1/1/1/1	-
3	EDO	M	202	-	-	0/1/1/1	-
3	EDO	J	202	-	-	0/1/1/1	-
3	EDO	G	202	-	-	0/1/1/1	-
3	EDO	H	203	-	-	1/1/1/1	-
3	EDO	A	203	-	-	0/1/1/1	-
3	EDO	M	203	-	-	0/1/1/1	-
3	EDO	K	203	-	-	0/1/1/1	-
2	CIT	L	201	-	-	0/6/16/16	-
3	EDO	N	202	-	-	0/1/1/1	-
3	EDO	I	202	-	-	1/1/1/1	-
3	EDO	H	204	-	-	0/1/1/1	-
2	CIT	K	201	-	-	0/6/16/16	-
2	CIT	E	201	-	-	0/6/16/16	-
2	CIT	F	201	-	-	0/6/16/16	-
3	EDO	F	202	-	-	0/1/1/1	-
3	EDO	E	202	-	-	0/1/1/1	-
2	CIT	A	201	-	-	1/6/16/16	-
3	EDO	O	202	-	-	0/1/1/1	-
3	EDO	B	202	-	-	0/1/1/1	-
2	CIT	H	202	-	-	0/6/16/16	-
2	CIT	D	201	-	-	0/6/16/16	-

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	CIT	C3-C2-C1	-4.11	108.40	114.98
2	L	201	CIT	C3-C4-C5	-4.09	108.44	114.98
2	J	201	CIT	C3-C2-C1	-3.92	108.71	114.98
2	C	201	CIT	C3-C2-C1	-3.86	108.80	114.98
2	D	201	CIT	C3-C2-C1	-3.78	108.93	114.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	CIT	C6-C3-C4-C5
3	H	203	EDO	O1-C1-C2-O2
3	L	202	EDO	O1-C1-C2-O2
3	I	202	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	204	EDO	1	0
2	A	201	CIT	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	140/149 (93%)	0.23	14 (10%) 7 6	26, 48, 80, 100	0
1	B	140/149 (93%)	-0.43	1 (0%) 87 88	21, 32, 51, 68	0
1	C	139/149 (93%)	-0.55	1 (0%) 87 88	17, 27, 47, 56	0
1	D	140/149 (93%)	-0.53	0 100 100	17, 28, 56, 76	0
1	E	139/149 (93%)	-0.51	2 (1%) 75 76	16, 25, 50, 62	0
1	F	141/149 (94%)	-0.47	2 (1%) 75 76	15, 25, 46, 85	0
1	G	141/149 (94%)	-0.43	2 (1%) 75 76	17, 28, 50, 75	0
1	H	141/149 (94%)	-0.22	3 (2%) 63 63	17, 30, 58, 85	0
1	I	140/149 (93%)	-0.61	1 (0%) 87 88	15, 25, 42, 49	0
1	J	141/149 (94%)	-0.32	1 (0%) 87 88	15, 25, 46, 65	0
1	K	140/149 (93%)	-0.37	1 (0%) 87 88	15, 25, 54, 65	0
1	L	141/149 (94%)	-0.36	1 (0%) 87 88	14, 22, 44, 83	0
1	M	141/149 (94%)	-0.47	5 (3%) 44 41	15, 26, 54, 75	0
1	N	141/149 (94%)	-0.28	7 (4%) 28 27	17, 31, 62, 81	0
1	O	139/149 (93%)	0.29	20 (14%) 2 2	23, 42, 72, 90	0
1	P	141/149 (94%)	-0.28	5 (3%) 44 41	22, 32, 61, 92	0
All	All	2245/2384 (94%)	-0.33	66 (2%) 51 50	14, 29, 60, 100	0

The worst 5 of 66 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	96	THR	6.6
1	O	59	PHE	5.5
1	A	2	ALA	5.4
1	G	1	MET	4.7
1	A	59	PHE	4.5

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	C	203	4/4	0.84	0.14	43,44,45,47	0
3	EDO	H	204	4/4	0.86	0.18	40,50,51,52	0
3	EDO	A	203	4/4	0.87	0.19	55,56,62,71	0
2	CIT	O	201	13/13	0.89	0.22	46,52,64,65	0
3	EDO	P	202	4/4	0.90	0.12	46,46,53,54	0
2	CIT	L	201	13/13	0.90	0.11	25,33,43,48	0
3	EDO	M	202	4/4	0.90	0.11	35,39,40,42	0
2	CIT	A	201	13/13	0.90	0.18	55,64,80,82	0
3	EDO	M	203	4/4	0.91	0.15	49,52,57,61	0
3	EDO	L	202	4/4	0.91	0.11	43,47,47,48	0
3	EDO	H	201	4/4	0.92	0.14	46,46,50,51	0
3	EDO	A	202	4/4	0.92	0.15	44,45,51,58	0
3	EDO	D	202	4/4	0.92	0.11	39,40,43,45	0
3	EDO	B	202	4/4	0.93	0.11	45,45,46,49	0
3	EDO	H	203	4/4	0.94	0.08	34,36,37,40	0
2	CIT	N	201	13/13	0.94	0.12	29,36,49,51	0
2	CIT	C	201	13/13	0.94	0.10	22,24,31,36	0
2	CIT	H	202	13/13	0.94	0.12	33,38,48,48	0
2	CIT	D	201	13/13	0.94	0.09	27,32,39,41	0
3	EDO	J	202	4/4	0.95	0.11	38,39,40,47	0
3	EDO	O	202	4/4	0.95	0.09	41,46,46,49	0
3	EDO	N	202	4/4	0.95	0.07	39,41,41,42	0
3	EDO	G	202	4/4	0.95	0.08	36,36,42,47	0
2	CIT	B	201	13/13	0.96	0.09	20,29,41,43	0
2	CIT	I	201	13/13	0.96	0.08	25,28,36,38	0
3	EDO	I	202	4/4	0.96	0.10	33,33,33,37	0
2	CIT	M	201	13/13	0.96	0.10	25,28,40,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CIT	E	201	13/13	0.96	0.09	25,29,40,43	0
2	CIT	F	201	13/13	0.96	0.11	21,27,34,36	0
3	EDO	E	202	4/4	0.96	0.08	35,36,39,40	0
3	EDO	C	202	4/4	0.96	0.06	32,34,35,36	0
2	CIT	G	201	13/13	0.96	0.10	20,24,36,37	0
3	EDO	K	202	4/4	0.96	0.08	35,36,37,39	0
2	CIT	P	201	13/13	0.96	0.10	25,31,44,45	0
2	CIT	J	201	13/13	0.97	0.05	21,24,33,35	0
2	CIT	K	201	13/13	0.97	0.10	24,28,38,42	0
3	EDO	K	203	4/4	0.97	0.10	27,28,34,40	0
3	EDO	F	202	4/4	0.98	0.06	33,33,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.