Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 11:41 PM EDT

PDB ID	:	4O0N
Title	:	2.4 Angstrom Resolution Crystal Structure of Putative Nucleoside Diphosphate Kinase from Toxoplasma gondii.
Authors	:	Minasov, G.; Ruan, J.; Ngo, H.; Shuvalova, L.; Dubrovska, I.; Flores, K.; Shanmugam, D.; Roos, D.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2013-12-13
Resolution	:	2.40 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

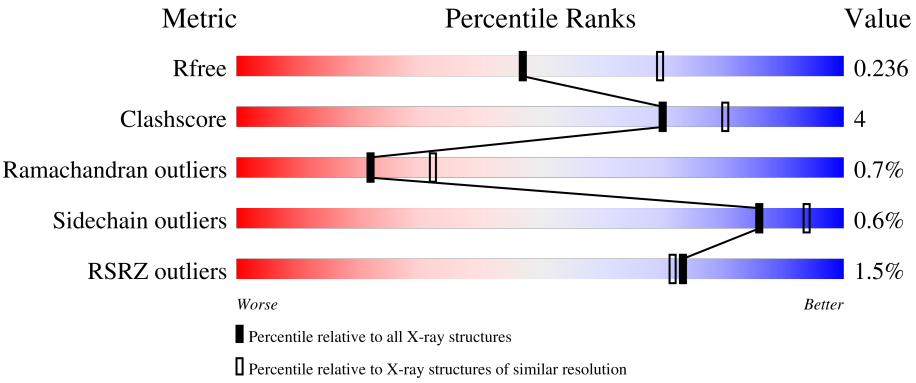
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	171	81% 8% • 11%
1	B	171	83% 6% • 10%
1	C	171	78% 11% 11%
1	D	171	84% 6% 10%

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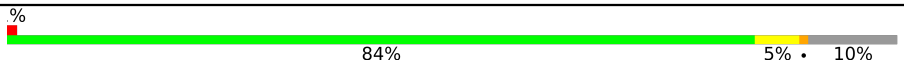
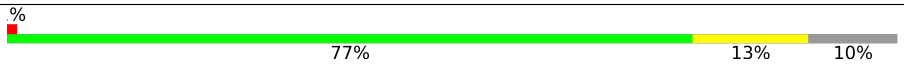
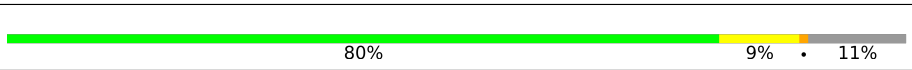
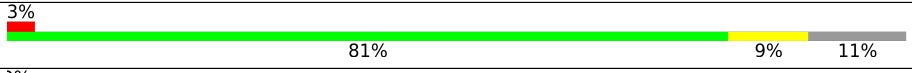
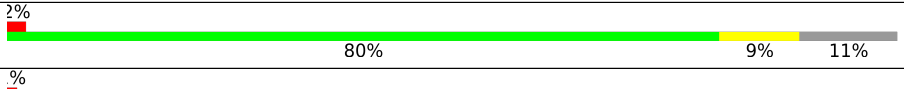
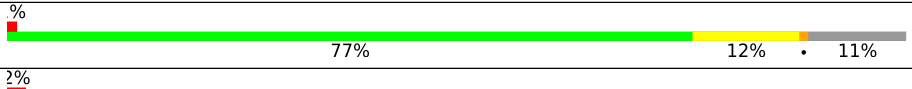
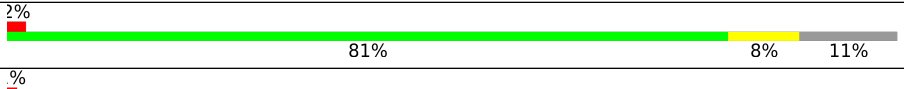
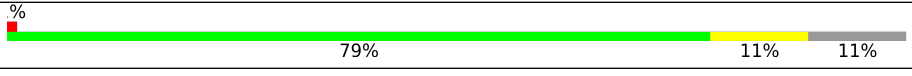
Mol	Chain	Length	Quality of chain
1	E	171	
1	F	171	
1	G	171	
1	H	171	
1	I	171	
1	J	171	
1	K	171	
1	L	171	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15516 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	153	Total	C	N	O	S	0	3	0
			1255	792	223	232	8			
1	B	154	Total	C	N	O	S	0	2	0
			1248	788	220	232	8			
1	C	153	Total	C	N	O	S	0	3	0
			1253	791	220	234	8			
1	D	154	Total	C	N	O	S	0	0	0
			1228	777	214	229	8			
1	E	154	Total	C	N	O	S	0	1	0
			1239	783	218	230	8			
1	F	154	Total	C	N	O	S	0	4	0
			1266	798	222	238	8			
1	G	152	Total	C	N	O	S	0	1	0
			1230	778	216	228	8			
1	H	153	Total	C	N	O	S	0	1	0
			1233	780	215	230	8			
1	I	153	Total	C	N	O	S	0	2	0
			1246	787	221	230	8			
1	J	153	Total	C	N	O	S	0	1	0
			1233	780	214	231	8			
1	K	153	Total	C	N	O	S	0	0	0
			1224	775	213	228	8			
1	L	153	Total	C	N	O	S	0	1	0
			1235	781	217	229	8			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLY	-	expression tag	UNP S8FF85
A	157	GLU	-	expression tag	UNP S8FF85
A	158	ASN	-	expression tag	UNP S8FF85
A	159	LEU	-	expression tag	UNP S8FF85
A	160	TYR	-	expression tag	UNP S8FF85

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Chain	Residue	Modelled	Actual	Comment	Reference
A	161	PHE	-	expression tag	UNP S8FF85
A	162	GLN	-	expression tag	UNP S8FF85
A	163	SER	-	expression tag	UNP S8FF85
A	164	ALA	-	expression tag	UNP S8FF85
A	165	GLY	-	expression tag	UNP S8FF85
A	166	HIS	-	expression tag	UNP S8FF85
A	167	HIS	-	expression tag	UNP S8FF85
A	168	HIS	-	expression tag	UNP S8FF85
A	169	HIS	-	expression tag	UNP S8FF85
A	170	HIS	-	expression tag	UNP S8FF85
A	171	HIS	-	expression tag	UNP S8FF85
B	156	GLY	-	expression tag	UNP S8FF85
B	157	GLU	-	expression tag	UNP S8FF85
B	158	ASN	-	expression tag	UNP S8FF85
B	159	LEU	-	expression tag	UNP S8FF85
B	160	TYR	-	expression tag	UNP S8FF85
B	161	PHE	-	expression tag	UNP S8FF85
B	162	GLN	-	expression tag	UNP S8FF85
B	163	SER	-	expression tag	UNP S8FF85
B	164	ALA	-	expression tag	UNP S8FF85
B	165	GLY	-	expression tag	UNP S8FF85
B	166	HIS	-	expression tag	UNP S8FF85
B	167	HIS	-	expression tag	UNP S8FF85
B	168	HIS	-	expression tag	UNP S8FF85
B	169	HIS	-	expression tag	UNP S8FF85
B	170	HIS	-	expression tag	UNP S8FF85
B	171	HIS	-	expression tag	UNP S8FF85
C	156	GLY	-	expression tag	UNP S8FF85
C	157	GLU	-	expression tag	UNP S8FF85
C	158	ASN	-	expression tag	UNP S8FF85
C	159	LEU	-	expression tag	UNP S8FF85
C	160	TYR	-	expression tag	UNP S8FF85
C	161	PHE	-	expression tag	UNP S8FF85
C	162	GLN	-	expression tag	UNP S8FF85
C	163	SER	-	expression tag	UNP S8FF85
C	164	ALA	-	expression tag	UNP S8FF85
C	165	GLY	-	expression tag	UNP S8FF85
C	166	HIS	-	expression tag	UNP S8FF85
C	167	HIS	-	expression tag	UNP S8FF85
C	168	HIS	-	expression tag	UNP S8FF85
C	169	HIS	-	expression tag	UNP S8FF85
C	170	HIS	-	expression tag	UNP S8FF85

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Chain	Residue	Modelled	Actual	Comment	Reference
C	171	HIS	-	expression tag	UNP S8FF85
D	156	GLY	-	expression tag	UNP S8FF85
D	157	GLU	-	expression tag	UNP S8FF85
D	158	ASN	-	expression tag	UNP S8FF85
D	159	LEU	-	expression tag	UNP S8FF85
D	160	TYR	-	expression tag	UNP S8FF85
D	161	PHE	-	expression tag	UNP S8FF85
D	162	GLN	-	expression tag	UNP S8FF85
D	163	SER	-	expression tag	UNP S8FF85
D	164	ALA	-	expression tag	UNP S8FF85
D	165	GLY	-	expression tag	UNP S8FF85
D	166	HIS	-	expression tag	UNP S8FF85
D	167	HIS	-	expression tag	UNP S8FF85
D	168	HIS	-	expression tag	UNP S8FF85
D	169	HIS	-	expression tag	UNP S8FF85
D	170	HIS	-	expression tag	UNP S8FF85
D	171	HIS	-	expression tag	UNP S8FF85
E	156	GLY	-	expression tag	UNP S8FF85
E	157	GLU	-	expression tag	UNP S8FF85
E	158	ASN	-	expression tag	UNP S8FF85
E	159	LEU	-	expression tag	UNP S8FF85
E	160	TYR	-	expression tag	UNP S8FF85
E	161	PHE	-	expression tag	UNP S8FF85
E	162	GLN	-	expression tag	UNP S8FF85
E	163	SER	-	expression tag	UNP S8FF85
E	164	ALA	-	expression tag	UNP S8FF85
E	165	GLY	-	expression tag	UNP S8FF85
E	166	HIS	-	expression tag	UNP S8FF85
E	167	HIS	-	expression tag	UNP S8FF85
E	168	HIS	-	expression tag	UNP S8FF85
E	169	HIS	-	expression tag	UNP S8FF85
E	170	HIS	-	expression tag	UNP S8FF85
E	171	HIS	-	expression tag	UNP S8FF85
F	156	GLY	-	expression tag	UNP S8FF85
F	157	GLU	-	expression tag	UNP S8FF85
F	158	ASN	-	expression tag	UNP S8FF85
F	159	LEU	-	expression tag	UNP S8FF85
F	160	TYR	-	expression tag	UNP S8FF85
F	161	PHE	-	expression tag	UNP S8FF85
F	162	GLN	-	expression tag	UNP S8FF85
F	163	SER	-	expression tag	UNP S8FF85
F	164	ALA	-	expression tag	UNP S8FF85

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Chain	Residue	Modelled	Actual	Comment	Reference
F	165	GLY	-	expression tag	UNP S8FF85
F	166	HIS	-	expression tag	UNP S8FF85
F	167	HIS	-	expression tag	UNP S8FF85
F	168	HIS	-	expression tag	UNP S8FF85
F	169	HIS	-	expression tag	UNP S8FF85
F	170	HIS	-	expression tag	UNP S8FF85
F	171	HIS	-	expression tag	UNP S8FF85
G	156	GLY	-	expression tag	UNP S8FF85
G	157	GLU	-	expression tag	UNP S8FF85
G	158	ASN	-	expression tag	UNP S8FF85
G	159	LEU	-	expression tag	UNP S8FF85
G	160	TYR	-	expression tag	UNP S8FF85
G	161	PHE	-	expression tag	UNP S8FF85
G	162	GLN	-	expression tag	UNP S8FF85
G	163	SER	-	expression tag	UNP S8FF85
G	164	ALA	-	expression tag	UNP S8FF85
G	165	GLY	-	expression tag	UNP S8FF85
G	166	HIS	-	expression tag	UNP S8FF85
G	167	HIS	-	expression tag	UNP S8FF85
G	168	HIS	-	expression tag	UNP S8FF85
G	169	HIS	-	expression tag	UNP S8FF85
G	170	HIS	-	expression tag	UNP S8FF85
G	171	HIS	-	expression tag	UNP S8FF85
H	156	GLY	-	expression tag	UNP S8FF85
H	157	GLU	-	expression tag	UNP S8FF85
H	158	ASN	-	expression tag	UNP S8FF85
H	159	LEU	-	expression tag	UNP S8FF85
H	160	TYR	-	expression tag	UNP S8FF85
H	161	PHE	-	expression tag	UNP S8FF85
H	162	GLN	-	expression tag	UNP S8FF85
H	163	SER	-	expression tag	UNP S8FF85
H	164	ALA	-	expression tag	UNP S8FF85
H	165	GLY	-	expression tag	UNP S8FF85
H	166	HIS	-	expression tag	UNP S8FF85
H	167	HIS	-	expression tag	UNP S8FF85
H	168	HIS	-	expression tag	UNP S8FF85
H	169	HIS	-	expression tag	UNP S8FF85
H	170	HIS	-	expression tag	UNP S8FF85
H	171	HIS	-	expression tag	UNP S8FF85
I	156	GLY	-	expression tag	UNP S8FF85
I	157	GLU	-	expression tag	UNP S8FF85
I	158	ASN	-	expression tag	UNP S8FF85

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Chain	Residue	Modelled	Actual	Comment	Reference
I	159	LEU	-	expression tag	UNP S8FF85
I	160	TYR	-	expression tag	UNP S8FF85
I	161	PHE	-	expression tag	UNP S8FF85
I	162	GLN	-	expression tag	UNP S8FF85
I	163	SER	-	expression tag	UNP S8FF85
I	164	ALA	-	expression tag	UNP S8FF85
I	165	GLY	-	expression tag	UNP S8FF85
I	166	HIS	-	expression tag	UNP S8FF85
I	167	HIS	-	expression tag	UNP S8FF85
I	168	HIS	-	expression tag	UNP S8FF85
I	169	HIS	-	expression tag	UNP S8FF85
I	170	HIS	-	expression tag	UNP S8FF85
I	171	HIS	-	expression tag	UNP S8FF85
J	156	GLY	-	expression tag	UNP S8FF85
J	157	GLU	-	expression tag	UNP S8FF85
J	158	ASN	-	expression tag	UNP S8FF85
J	159	LEU	-	expression tag	UNP S8FF85
J	160	TYR	-	expression tag	UNP S8FF85
J	161	PHE	-	expression tag	UNP S8FF85
J	162	GLN	-	expression tag	UNP S8FF85
J	163	SER	-	expression tag	UNP S8FF85
J	164	ALA	-	expression tag	UNP S8FF85
J	165	GLY	-	expression tag	UNP S8FF85
J	166	HIS	-	expression tag	UNP S8FF85
J	167	HIS	-	expression tag	UNP S8FF85
J	168	HIS	-	expression tag	UNP S8FF85
J	169	HIS	-	expression tag	UNP S8FF85
J	170	HIS	-	expression tag	UNP S8FF85
J	171	HIS	-	expression tag	UNP S8FF85
K	156	GLY	-	expression tag	UNP S8FF85
K	157	GLU	-	expression tag	UNP S8FF85
K	158	ASN	-	expression tag	UNP S8FF85
K	159	LEU	-	expression tag	UNP S8FF85
K	160	TYR	-	expression tag	UNP S8FF85
K	161	PHE	-	expression tag	UNP S8FF85
K	162	GLN	-	expression tag	UNP S8FF85
K	163	SER	-	expression tag	UNP S8FF85
K	164	ALA	-	expression tag	UNP S8FF85
K	165	GLY	-	expression tag	UNP S8FF85
K	166	HIS	-	expression tag	UNP S8FF85
K	167	HIS	-	expression tag	UNP S8FF85
K	168	HIS	-	expression tag	UNP S8FF85

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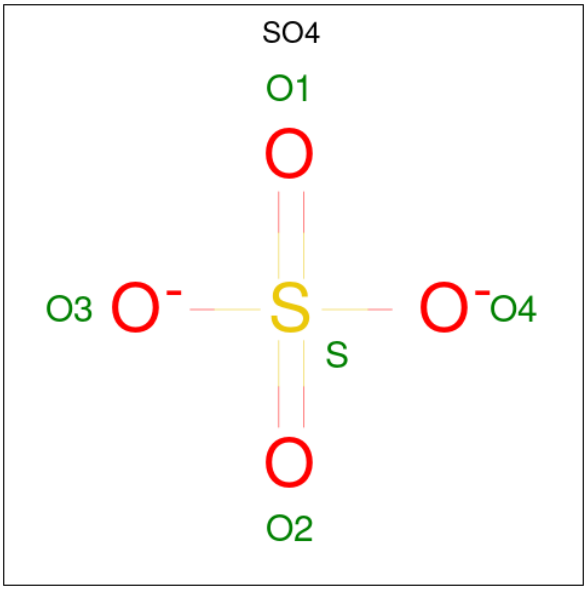
Chain	Residue	Modelled	Actual	Comment	Reference
K	169	HIS	-	expression tag	UNP S8FF85
K	170	HIS	-	expression tag	UNP S8FF85
K	171	HIS	-	expression tag	UNP S8FF85
L	156	GLY	-	expression tag	UNP S8FF85
L	157	GLU	-	expression tag	UNP S8FF85
L	158	ASN	-	expression tag	UNP S8FF85
L	159	LEU	-	expression tag	UNP S8FF85
L	160	TYR	-	expression tag	UNP S8FF85
L	161	PHE	-	expression tag	UNP S8FF85
L	162	GLN	-	expression tag	UNP S8FF85
L	163	SER	-	expression tag	UNP S8FF85
L	164	ALA	-	expression tag	UNP S8FF85
L	165	GLY	-	expression tag	UNP S8FF85
L	166	HIS	-	expression tag	UNP S8FF85
L	167	HIS	-	expression tag	UNP S8FF85
L	168	HIS	-	expression tag	UNP S8FF85
L	169	HIS	-	expression tag	UNP S8FF85
L	170	HIS	-	expression tag	UNP S8FF85
L	171	HIS	-	expression tag	UNP S8FF85

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	K	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	57	Total O 58 58	0	1
3	B	71	Total O 72 72	0	2
3	C	70	Total O 71 71	0	2
3	D	33	Total O 33 33	0	0
3	E	53	Total O 55 55	0	2
3	F	75	Total O 76 76	0	2
3	G	55	Total O 56 56	0	2

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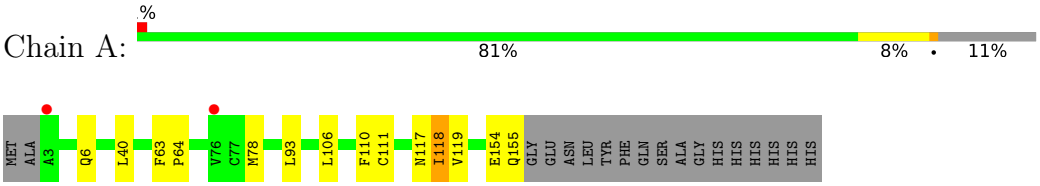
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	34	Total O 34 34	0	0
3	I	25	Total O 25 25	0	0
3	J	24	Total O 24 24	0	1
3	K	32	Total O 33 33	0	1
3	L	19	Total O 19 19	0	0

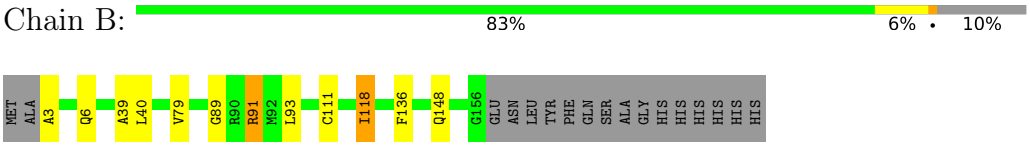
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

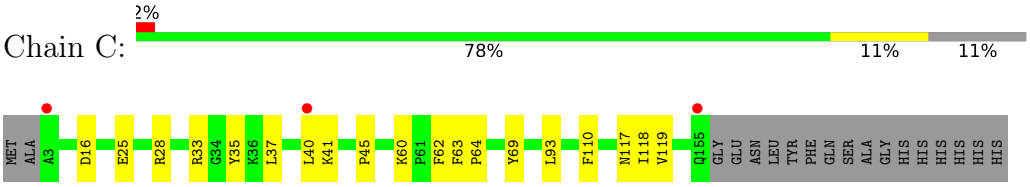
• Molecule 1: Nucleoside diphosphate kinase



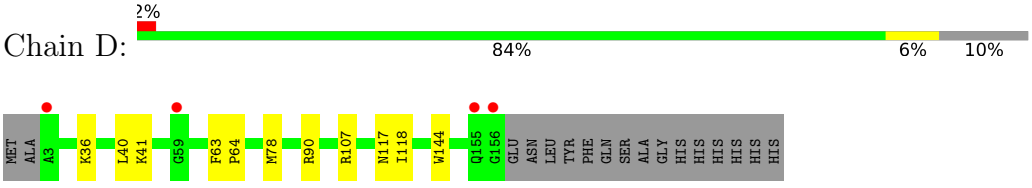
• Molecule 1: Nucleoside diphosphate kinase



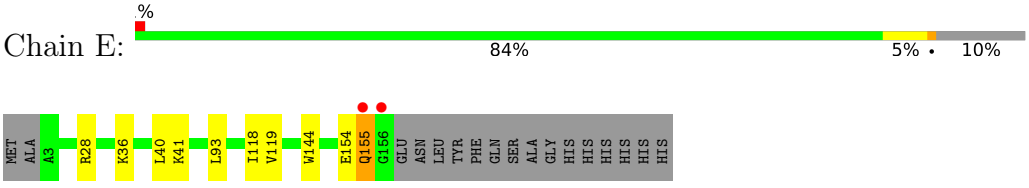
• Molecule 1: Nucleoside diphosphate kinase



• Molecule 1: Nucleoside diphosphate kinase

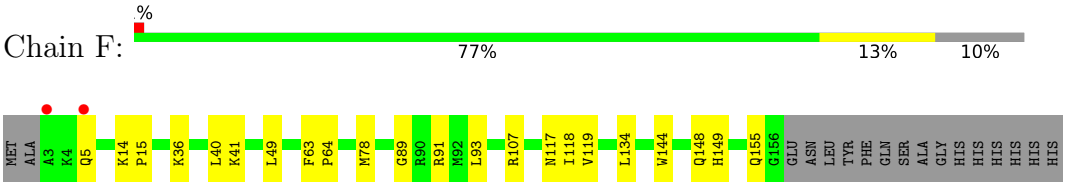


• Molecule 1: Nucleoside diphosphate kinase



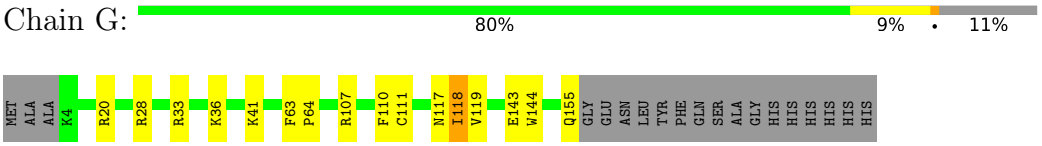
• Molecule 1: Nucleoside diphosphate kinase

Chain F:



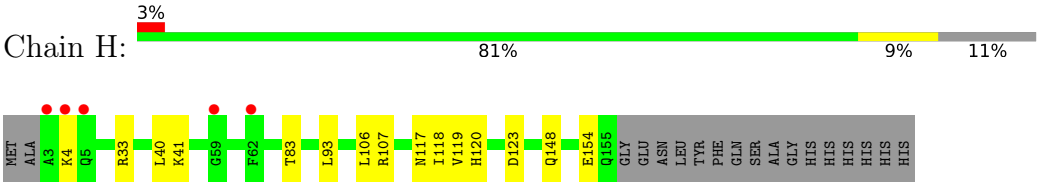
• Molecule 1: Nucleoside diphosphate kinase

Chain G:



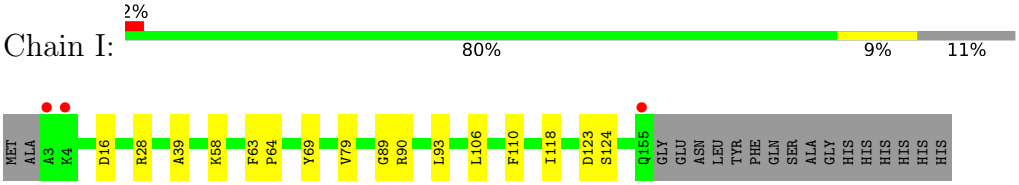
• Molecule 1: Nucleoside diphosphate kinase

Chain H:



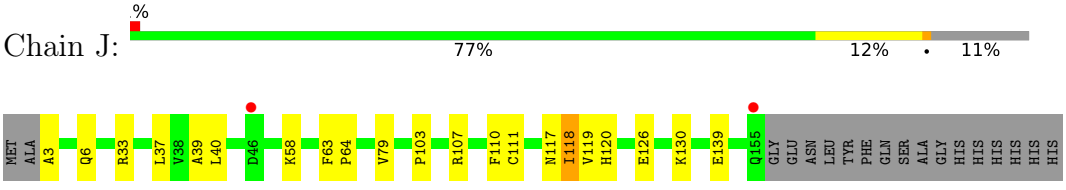
• Molecule 1: Nucleoside diphosphate kinase

Chain I:



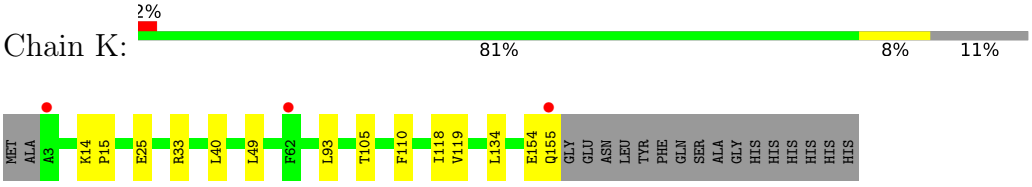
• Molecule 1: Nucleoside diphosphate kinase

Chain J:



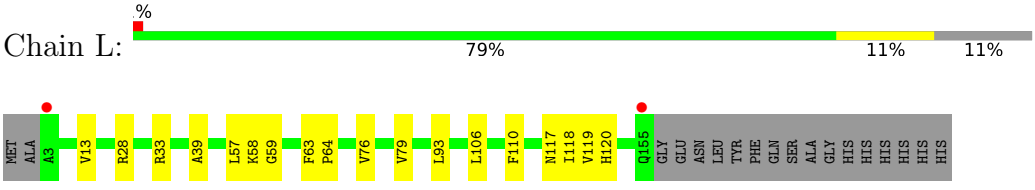
• Molecule 1: Nucleoside diphosphate kinase

Chain K:



• Molecule 1: Nucleoside diphosphate kinase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.39Å 121.59Å 212.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.49 – 2.40 29.49 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.49-2.40) 99.6 (29.49-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.07 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.192 , 0.238 0.194 , 0.236	Depositor DCC
R_{free} test set	3771 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	41.4	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15516	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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, 0.333 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: SO4

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	0/1283	0.63	0/1731
1	B	0.40	0/1276	0.65	0/1722
1	C	0.41	0/1281	0.62	0/1729
1	D	0.37	0/1256	0.62	0/1696
1	E	0.37	0/1267	0.63	0/1710
1	F	0.39	0/1294	0.63	0/1746
1	G	0.38	0/1258	0.59	0/1698
1	H	0.36	0/1261	0.59	0/1703
1	I	0.34	0/1274	0.55	0/1719
1	J	0.35	0/1261	0.58	0/1703
1	K	0.34	0/1252	0.58	0/1691
1	L	0.33	0/1263	0.56	0/1705
All	All	0.37	0/15226	0.60	0/20553

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	1255	0	1242	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1248	0	1233	8	0
1	C	1253	0	1237	18	0
1	D	1228	0	1214	5	0
1	E	1239	0	1226	6	0
1	F	1266	0	1243	13	0
1	G	1230	0	1218	11	0
1	H	1233	0	1218	12	0
1	I	1246	0	1235	10	0
1	J	1233	0	1216	14	0
1	K	1224	0	1211	9	0
1	L	1235	0	1223	12	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	10	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	1	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
3	A	58	0	0	0	0
3	B	72	0	0	1	0
3	C	71	0	0	1	0
3	D	33	0	0	0	0
3	E	55	0	0	0	0
3	F	76	0	0	2	0
3	G	56	0	0	0	0
3	H	34	0	0	0	0
3	I	25	0	0	0	0
3	J	24	0	0	0	0
3	K	33	0	0	0	0
3	L	19	0	0	0	0
All	All	15516	0	14716	108	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 (108) 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:J:126[A]:GLU:N	1:J:126[A]:GLU:OE2	2.19	0.76
1:I:28[A]:ARG:HH21	1:L:28[A]:ARG:HE	1.42	0.67
1:A:111:CYS:SG	1:A:118:ILE:HG12	2.38	0.64
1:L:58:LYS:N	1:L:59:GLY:HA3	2.14	0.63
1:A:154:GLU:HA	1:A:155:GLN:HB3	1.82	0.60
1:I:39:ALA:HB3	1:I:79:VAL:HB	1.84	0.59
1:F:5:GLN:OE1	1:F:149:HIS:NE2	2.38	0.56
1:C:93:LEU:HD22	1:C:119:VAL:HG11	1.88	0.56
1:L:39:ALA:HB3	1:L:79:VAL:HB	1.89	0.55
1:K:49:LEU:HD11	1:K:134:LEU:HG	1.90	0.54
1:J:103:PRO:HG2	1:K:105:THR:HG22	1.90	0.54
1:J:63:PHE:HB3	1:J:64:PRO:HD3	1.89	0.53
1:J:3:ALA:HB3	1:J:6:GLN:HG2	1.91	0.53
1:C:45:PRO:HD2	3:C:312:HOH:O	2.09	0.52
1:G:20:ARG:HG2	1:H:148[B]:GLN:CG	2.39	0.52
1:I:28[A]:ARG:HE	1:L:28[A]:ARG:HH21	1.57	0.52
1:G:36:LYS:HG3	1:G:144:TRP:CZ2	2.45	0.52
1:L:57:LEU:O	1:L:63:PHE:CD1	2.62	0.52
1:A:110:PHE:HA	1:C:33[B]:ARG:HA	1.91	0.51
1:E:93:LEU:HD22	1:E:119:VAL:HG11	1.93	0.51
1:F:89:GLY:O	1:F:93:LEU:HG	2.11	0.51
1:J:120:HIS:ND1	2:J:201:SO4:O3	2.36	0.50
1:J:107:ARG:HD3	1:J:117:ASN:HB2	1.93	0.50
1:C:33[B]:ARG:HG2	1:C:35:TYR:CE2	2.47	0.50
1:K:154:GLU:O	1:K:155:GLN:C	2.50	0.49
1:A:154:GLU:CA	1:A:155:GLN:HB3	2.43	0.49
1:C:37:LEU:HD21	1:C:40:LEU:HD22	1.95	0.49
1:B:148:GLN:HE21	1:B:148:GLN:HA	1.78	0.48
1:B:89:GLY:O	1:B:93:LEU:HG	2.13	0.48
1:D:63:PHE:HB3	1:D:64:PRO:HD3	1.96	0.48
1:K:93:LEU:HD22	1:K:119:VAL:HG11	1.94	0.48
1:G:107:ARG:HD3	1:G:117:ASN:HB2	1.94	0.48
1:J:33:ARG:HA	1:L:110:PHE:HA	1.96	0.48
1:A:93:LEU:HD23	1:A:106:LEU:HD12	1.96	0.48
1:D:40:LEU:HD13	1:D:78:MET:HG2	1.96	0.48
1:E:154:GLU:O	1:E:155:GLN:C	2.52	0.48
1:L:63:PHE:HB3	1:L:64:PRO:HD3	1.95	0.48
1:I:16:ASP:OD1	1:I:69:TYR:OH	2.31	0.48
1:B:91:ARG:HD2	3:B:364:HOH:O	2.14	0.48
1:H:117:ASN:O	1:H:119:VAL:N	2.42	0.47
1:A:63:PHE:HB3	1:A:64:PRO:HD3	1.96	0.47
1:C:28:ARG:HH21	1:E:28[A]:ARG:HE	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:PHE:HA	1:H:33:ARG:HA	1.97	0.47
1:C:33[B]:ARG:O	1:C:33[B]:ARG:HG3	2.15	0.47
1:C:93:LEU:HD22	1:C:119:VAL:CG1	2.45	0.47
1:I:89:GLY:O	1:I:93:LEU:HG	2.14	0.46
1:G:63:PHE:HB3	1:G:64:PRO:HD3	1.98	0.46
1:J:117:ASN:O	1:J:119:VAL:N	2.46	0.46
1:A:111:CYS:O	1:C:33[B]:ARG:HD2	2.15	0.46
1:H:41:LYS:HA	1:J:40:LEU:O	2.15	0.46
1:I:63:PHE:HB3	1:I:64:PRO:HD3	1.97	0.46
1:K:14:LYS:HB3	1:K:15:PRO:CD	2.46	0.46
1:F:117:ASN:O	1:F:119:VAL:N	2.44	0.45
1:F:63:PHE:HB3	1:F:64:PRO:HD3	1.98	0.45
1:L:13:VAL:HB	1:L:76:VAL:HB	1.98	0.45
1:B:79:VAL:HG23	1:B:136:PHE:CE2	2.52	0.45
1:C:33[B]:ARG:HG2	1:C:35:TYR:CD2	2.52	0.45
1:H:93:LEU:HD23	1:H:106:LEU:HD12	1.98	0.44
1:J:111:CYS:SG	1:J:118:ILE:HG23	2.57	0.44
1:C:60:LYS:HD3	1:C:62:PHE:CZ	2.52	0.44
1:H:93:LEU:HD22	1:H:119:VAL:HG11	1.99	0.44
1:K:110:PHE:HA	1:L:33:ARG:HA	1.99	0.44
1:B:3:ALA:HB3	1:B:6[A]:GLN:HE21	1.82	0.44
1:L:93:LEU:HD23	1:L:106:LEU:HD12	1.99	0.44
1:C:25:GLU:HG2	1:C:110:PHE:CZ	2.53	0.43
1:B:39:ALA:HB3	1:B:79:VAL:HB	2.00	0.43
1:D:107:ARG:HD3	1:D:117:ASN:HB2	2.00	0.43
1:J:39:ALA:HB3	1:J:79:VAL:HB	1.99	0.43
1:H:148[B]:GLN:HA	1:H:148[B]:GLN:OE1	2.17	0.43
1:F:40:LEU:HD13	1:F:78:MET:HG2	2.00	0.43
1:F:148[B]:GLN:NE2	3:F:341:HOH:O	2.51	0.43
1:C:117:ASN:O	1:C:119:VAL:N	2.48	0.42
1:H:40:LEU:HD21	1:J:40:LEU:HD11	2.00	0.42
1:F:93:LEU:O	1:F:107:ARG:HG3	2.20	0.42
1:H:119:VAL:HG22	1:H:120:HIS:N	2.35	0.42
1:F:91[B]:ARG:NH2	3:F:374[B]:HOH:O	2.50	0.42
1:H:107:ARG:HD3	1:H:117:ASN:HB2	2.01	0.42
1:C:63:PHE:HB3	1:C:64:PRO:HD3	2.00	0.42
1:G:111:CYS:SG	1:G:118:ILE:HG12	2.60	0.42
1:I:93:LEU:HD23	1:I:106:LEU:HD12	2.01	0.42
1:E:36:LYS:HG3	1:E:144:TRP:CZ2	2.54	0.42
1:G:117:ASN:O	1:G:119:VAL:N	2.50	0.42
1:A:40:LEU:O	1:D:41:LYS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PHE:HA	1:C:33[A]:ARG:HA	2.01	0.42
1:C:41:LYS:HA	1:E:40:LEU:O	2.19	0.42
1:G:41:LYS:HA	1:K:40:LEU:O	2.20	0.42
1:B:111:CYS:SG	1:B:118:ILE:HG23	2.60	0.41
1:C:40:LEU:O	1:E:41:LYS:HA	2.21	0.41
1:G:33:ARG:HA	1:I:110:PHE:HA	2.02	0.41
1:H:154:GLU:HG3	1:H:154:GLU:O	2.21	0.41
1:A:40:LEU:HD13	1:A:78:MET:HG2	2.01	0.41
1:G:28:ARG:NH1	1:K:25:GLU:OE1	2.47	0.41
1:I:123:ASP:OD1	1:I:124:SER:N	2.54	0.41
1:F:36:LYS:HG3	1:F:144:TRP:CZ2	2.56	0.41
1:F:49:LEU:HD11	1:F:134:LEU:HG	2.03	0.41
1:A:117:ASN:O	1:A:119:VAL:N	2.52	0.41
1:F:14:LYS:HB3	1:F:15:PRO:CD	2.51	0.41
1:G:143:GLU:HA	1:G:143:GLU:OE1	2.21	0.41
1:H:4:LYS:HB3	1:H:83:THR:HG23	2.03	0.41
1:J:37:LEU:HD21	1:J:40:LEU:HD22	2.03	0.41
1:J:110:PHE:HA	1:K:33:ARG:HA	2.03	0.41
1:L:117:ASN:O	1:L:119:VAL:N	2.50	0.41
1:D:36:LYS:HG3	1:D:144:TRP:CZ2	2.56	0.41
1:B:40:LEU:O	1:F:41:LYS:HA	2.21	0.40
1:I:90[A]:ARG:HD2	1:I:123:ASP:HA	2.03	0.40
1:F:5:GLN:OE1	1:F:149:HIS:CD2	2.74	0.40
1:L:119:VAL:HG22	1:L:120:HIS:N	2.37	0.40
1:C:16:ASP:OD1	1:C:69:TYR:OH	2.38	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	154/171 (90%)	151 (98%)	2 (1%)	1 (1%)	25 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	154/171 (90%)	151 (98%)	2 (1%)	1 (1%)	25	36
1	C	154/171 (90%)	151 (98%)	2 (1%)	1 (1%)	25	36
1	D	152/171 (89%)	147 (97%)	4 (3%)	1 (1%)	22	32
1	E	153/171 (90%)	151 (99%)	1 (1%)	1 (1%)	22	32
1	F	156/171 (91%)	152 (97%)	2 (1%)	2 (1%)	12	17
1	G	151/171 (88%)	148 (98%)	2 (1%)	1 (1%)	22	32
1	H	152/171 (89%)	147 (97%)	4 (3%)	1 (1%)	22	32
1	I	153/171 (90%)	147 (96%)	5 (3%)	1 (1%)	22	32
1	J	152/171 (89%)	145 (95%)	6 (4%)	1 (1%)	22	32
1	K	151/171 (88%)	148 (98%)	2 (1%)	1 (1%)	22	32
1	L	152/171 (89%)	146 (96%)	5 (3%)	1 (1%)	22	32
All	All	1834/2052 (89%)	1784 (97%)	37 (2%)	13 (1%)	22	32

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ILE
1	B	118	ILE
1	C	118	ILE
1	D	118	ILE
1	E	118	ILE
1	F	118	ILE
1	G	118	ILE
1	H	118	ILE
1	I	118	ILE
1	J	118	ILE
1	K	118	ILE
1	L	118	ILE
1	F	155	GLN

5.3.2 Protein sidechains (i)

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	137/148 (93%)	136 (99%)	1 (1%)	84 92
1	B	136/148 (92%)	135 (99%)	1 (1%)	84 92
1	C	137/148 (93%)	137 (100%)	0	100 100
1	D	134/148 (90%)	133 (99%)	1 (1%)	84 92
1	E	135/148 (91%)	134 (99%)	1 (1%)	84 92
1	F	138/148 (93%)	138 (100%)	0	100 100
1	G	135/148 (91%)	134 (99%)	1 (1%)	84 92
1	H	135/148 (91%)	134 (99%)	1 (1%)	84 92
1	I	136/148 (92%)	135 (99%)	1 (1%)	84 92
1	J	135/148 (91%)	132 (98%)	3 (2%)	52 71
1	K	134/148 (90%)	134 (100%)	0	100 100
1	L	135/148 (91%)	135 (100%)	0	100 100
All	All	1627/1776 (92%)	1617 (99%)	10 (1%)	86 94

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	B	91	ARG
1	D	90	ARG
1	E	155	GLN
1	G	155	GLN
1	H	123	ASP
1	I	58	LYS
1	J	58	LYS
1	J	130	LYS
1	J	139	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	155	GLN
1	B	148	GLN
1	C	155	GLN
1	E	32	GLN
1	E	149	HIS
1	G	155	GLN

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Mol	Chain	Res	Type
1	H	32	GLN
1	H	129	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 monosaccharides in this entry.

5.6 Ligand geometry

14 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	SO4	K	201	-	4,4,4	0.33	0	6,6,6	0.11	0
2	SO4	A	201	-	4,4,4	0.30	0	6,6,6	0.10	0
2	SO4	D	201	-	4,4,4	0.32	0	6,6,6	0.13	0
2	SO4	J	201	-	4,4,4	0.37	0	6,6,6	0.17	0
2	SO4	F	201	-	4,4,4	0.40	0	6,6,6	0.13	0
2	SO4	I	201	-	4,4,4	0.35	0	6,6,6	0.15	0
2	SO4	B	201	-	4,4,4	0.33	0	6,6,6	0.15	0
2	SO4	H	201	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	E	201	-	4,4,4	0.32	0	6,6,6	0.14	0
2	SO4	L	201	-	4,4,4	0.34	0	6,6,6	0.09	0
2	SO4	C	201	-	4,4,4	0.30	0	6,6,6	0.19	0
2	SO4	G	201	-	4,4,4	0.35	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	202	-	4,4,4	0.36	0	6,6,6	0.15	0
2	SO4	E	202	-	4,4,4	0.38	0	6,6,6	0.12	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	201	SO4	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^{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	153/171 (89%)	-0.41	2 (1%) 77 75	27, 40, 63, 92	0
1	B	154/171 (90%)	-0.56	0 100 100	24, 33, 58, 80	0
1	C	153/171 (89%)	-0.51	3 (1%) 65 63	24, 33, 57, 95	0
1	D	154/171 (90%)	-0.40	4 (2%) 56 54	30, 44, 65, 91	0
1	E	154/171 (90%)	-0.29	2 (1%) 77 75	28, 39, 74, 94	0
1	F	154/171 (90%)	-0.52	2 (1%) 77 75	24, 35, 57, 96	0
1	G	152/171 (88%)	-0.51	0 100 100	33, 40, 58, 81	0
1	H	153/171 (89%)	-0.16	5 (3%) 46 45	35, 54, 89, 122	0
1	I	153/171 (89%)	-0.09	3 (1%) 65 63	42, 57, 85, 111	0
1	J	153/171 (89%)	-0.11	2 (1%) 77 75	37, 59, 77, 115	0
1	K	153/171 (89%)	-0.22	3 (1%) 65 63	38, 51, 73, 101	0
1	L	153/171 (89%)	-0.01	2 (1%) 77 75	46, 64, 98, 117	0
All	All	1839/2052 (89%)	-0.31	28 (1%) 73 72	24, 46, 80, 122	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	156	GLY	7.7
1	H	3	ALA	5.2
1	H	59	GLY	5.1
1	J	155	GLN	4.7
1	I	3	ALA	4.2
1	A	3	ALA	4.0
1	C	3	ALA	3.8
1	L	155	GLN	3.8
1	H	62	PHE	3.6
1	H	5	GLN	3.4
1	D	155	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	4	LYS	3.2
1	E	155	GLN	3.0
1	L	3	ALA	2.9
1	F	5	GLN	2.7
1	J	46	ASP	2.7
1	K	3	ALA	2.6
1	F	3	ALA	2.6
1	I	155	GLN	2.6
1	D	59	GLY	2.6
1	K	155	GLN	2.6
1	D	156	GLY	2.5
1	A	76	VAL	2.3
1	C	155	GLN	2.1
1	C	40	LEU	2.1
1	D	3	ALA	2.1
1	K	62	PHE	2.1
1	H	4	LYS	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	SO4	E	202	5/5	0.83	0.24	46,49,51,51	5
2	SO4	L	201	5/5	0.84	0.32	53,55,59,61	5
2	SO4	J	201	5/5	0.87	0.16	67,82,85,90	0
2	SO4	I	201	5/5	0.93	0.13	80,81,84,87	0
2	SO4	K	201	5/5	0.94	0.12	88,98,102,102	0
2	SO4	H	201	5/5	0.94	0.10	75,77,83,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	F	201	5/5	0.95	0.12	60,61,71,73	0
2	SO4	B	202	5/5	0.95	0.19	62,70,78,80	0
2	SO4	A	201	5/5	0.96	0.10	60,61,69,71	0
2	SO4	E	201	5/5	0.97	0.08	62,69,76,76	0
2	SO4	B	201	5/5	0.97	0.09	55,58,62,66	0
2	SO4	G	201	5/5	0.98	0.07	51,54,65,65	0
2	SO4	D	201	5/5	0.98	0.08	63,63,69,69	0
2	SO4	C	201	5/5	0.98	0.10	59,62,65,67	0

6.5 Other polymers (i)

There are no such residues in this entry.