



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:02 PM GMT

PDB ID : 3ADC  
Title : Crystal structure of O-phosphoseryl-tRNA kinase complexed with selenocysteine tRNA and AMPPNP (crystal type 2)  
Authors : Itoh, Y.; Chiba, S.; Sekine, S.; Yokoyama, S.  
Deposited on : 2010-01-18  
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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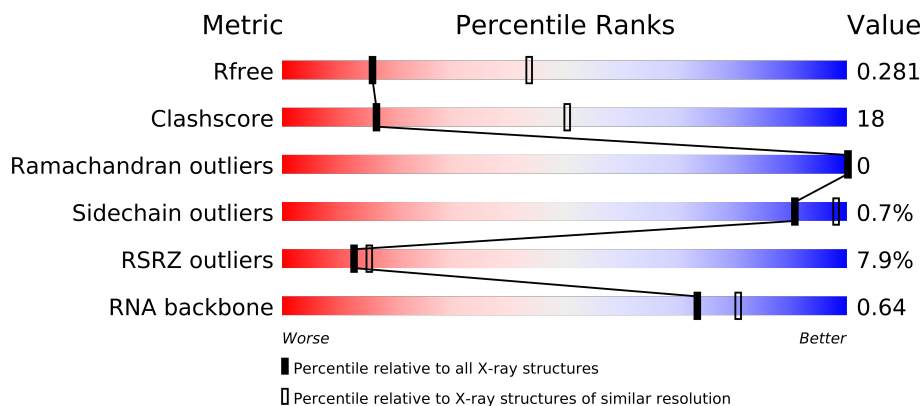
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	259	
1	B	259	
2	C	92	
2	D	92	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8023 atoms, of which 0 are hydrogen and 0 are deuterium.

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 L-seryl-tRNA(Sec) kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	Se	0	0	0
			2065	1339	341	381	4			
1	B	239	Total	C	N	O	Se	0	0	0
			2004	1301	332	367	4			

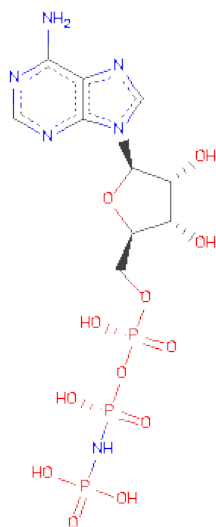
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MSE	-	EXPRESSION TAG	UNP Q58933
A	-9	ASN	-	EXPRESSION TAG	UNP Q58933
A	-8	HIS	-	EXPRESSION TAG	UNP Q58933
A	-7	LYS	-	EXPRESSION TAG	UNP Q58933
A	-6	VAL	-	EXPRESSION TAG	UNP Q58933
A	-5	HIS	-	EXPRESSION TAG	UNP Q58933
A	-4	HIS	-	EXPRESSION TAG	UNP Q58933
A	-3	HIS	-	EXPRESSION TAG	UNP Q58933
A	-2	HIS	-	EXPRESSION TAG	UNP Q58933
A	-1	HIS	-	EXPRESSION TAG	UNP Q58933
A	0	HIS	-	EXPRESSION TAG	UNP Q58933
B	-10	MSE	-	EXPRESSION TAG	UNP Q58933
B	-9	ASN	-	EXPRESSION TAG	UNP Q58933
B	-8	HIS	-	EXPRESSION TAG	UNP Q58933
B	-7	LYS	-	EXPRESSION TAG	UNP Q58933
B	-6	VAL	-	EXPRESSION TAG	UNP Q58933
B	-5	HIS	-	EXPRESSION TAG	UNP Q58933
B	-4	HIS	-	EXPRESSION TAG	UNP Q58933
B	-3	HIS	-	EXPRESSION TAG	UNP Q58933
B	-2	HIS	-	EXPRESSION TAG	UNP Q58933
B	-1	HIS	-	EXPRESSION TAG	UNP Q58933
B	0	HIS	-	EXPRESSION TAG	UNP Q58933

- Molecule 2 is a RNA chain called selenocysteine tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	88	Total	C	N	O	P	0	0	0
			1886	836	344	618	88			
2	D	92	Total	C	N	O	P	0	0	0
			1968	873	356	647	92			

- Molecule 3 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

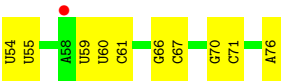
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	9	Total	O	0	0
			9	9		
5	C	9	Total	O	0	0
			9	9		
5	D	9	Total	O	0	0
			9	9		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.82Å 263.56Å 46.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.21 – 2.90 28.21 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.3 (28.21-2.90) 95.4 (28.21-2.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.224 , 0.277 0.227 , 0.281	Depositor DCC
$R_{free}$ test set	1326 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	84.4	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 25842 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8023	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	112.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

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

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	0.35	0/2095	0.58	0/2796
1	B	0.35	0/2033	0.56	0/2711
2	C	0.44	1/2104 (0.0%)	0.69	0/3278
2	D	0.36	1/2196 (0.0%)	0.71	0/3423
All	All	0.38	2/8428 (0.0%)	0.64	0/12208

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	G	OP3-P	-7.19	1.52	1.61
2	D	1	G	OP3-P	-7.12	1.52	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2065	0	2165	71	0
1	B	2004	0	2112	87	0
2	C	1886	0	962	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1968	0	1003	66	0
3	A	31	0	13	7	0
3	B	31	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	9	0	0	0	0
5	B	9	0	0	0	0
5	C	9	0	0	0	0
5	D	9	0	0	1	0
All	All	8023	0	6268	254	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (254) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:192:LYS:HE2	2:D:16:U:H5'	1.40	1.03
1:A:116:ARG:HH21	3:A:2001:ANP:H5'2	1.23	1.00
2:C:31:A:H2'	2:C:32:C:O4'	1.76	0.85
1:A:116:ARG:HH22	3:A:2001:ANP:HNB1	1.19	0.85
1:A:0:HIS:HB2	1:A:70:TRP:CD1	2.14	0.82
2:D:47(E):G:H3'	2:D:47(F):A:H5''	1.62	0.81
1:B:0:HIS:HA	1:B:70:TRP:NE1	1.96	0.80
2:C:59:U:O2'	2:C:60:U:H5'	1.85	0.77
2:D:47(E):G:H2'	2:D:47(G):G:H5''	1.67	0.76
2:C:7:C:H5''	2:C:8:C:H5'	1.68	0.76
1:B:217:GLU:O	1:B:221:GLU:HG2	1.86	0.76
1:A:116:ARG:NH2	3:A:2001:ANP:H5'2	1.98	0.76
1:A:8:LEU:HD11	1:A:129:TYR:HA	1.68	0.75
2:C:37:G:H2'	2:C:38:A:C8	2.21	0.75
1:B:219:ARG:NH1	1:B:223:LEU:HD11	2.02	0.74
1:B:121:PRO:HG2	1:B:124:VAL:HG23	1.68	0.73
2:D:59:U:O2'	2:D:60:U:H5'	1.89	0.73
1:B:84:ARG:HD2	5:D:1014:HOH:O	1.88	0.72
2:D:47(C):C:H2'	2:D:47(D):C:C6	2.24	0.72
1:B:121:PRO:HG2	1:B:124:VAL:CG2	2.18	0.72
1:B:202:ILE:HD12	2:D:19:G:C6	2.26	0.71
1:B:226:ILE:HD13	1:B:237:VAL:HG11	1.72	0.71
2:D:43:G:O2'	2:D:44:C:H5'	1.91	0.71
1:B:121:PRO:HB2	1:B:123:GLU:HG2	1.74	0.70
1:A:121:PRO:HG2	1:A:124:VAL:HG23	1.74	0.70
2:C:32:C:N3	2:C:38:A:N6	2.39	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:36:A:H2'	2:D:37:G:C8	2.26	0.70
1:A:78:TYR:HB2	1:A:132:PHE:HD1	1.57	0.70
1:B:195:ARG:NH1	2:D:19:G:H3'	2.06	0.70
1:A:175:VAL:CG1	1:A:176:LEU:N	2.54	0.69
1:A:116:ARG:HH21	3:A:2001:ANP:C5'	2.00	0.69
1:A:11:VAL:O	1:A:150:THR:HG21	1.92	0.69
2:C:38:A:O5'	2:C:38:A:H8	1.76	0.68
2:D:47(E):G:H5''	2:D:47(F):A:OP2	1.93	0.68
2:D:23:C:H2'	2:D:24:G:H8	1.59	0.68
1:A:175:VAL:HG12	1:A:176:LEU:N	2.08	0.68
1:B:160:ALA:O	1:B:164:ILE:HG13	1.94	0.68
1:B:232:VAL:HG13	1:B:237:VAL:HG21	1.76	0.67
1:A:121:PRO:HG2	1:A:124:VAL:CG2	2.24	0.67
2:D:7:C:H5''	2:D:8:C:H5'	1.75	0.67
1:A:222:PHE:CZ	1:A:226:ILE:HD11	2.30	0.67
2:C:37:G:H2'	2:C:38:A:N7	2.09	0.67
2:C:31:A:H2'	2:C:32:C:C4'	2.25	0.66
2:C:43:G:O2'	2:C:44:C:H5'	1.95	0.66
2:C:72:C:O2'	2:C:73:G:H5'	1.96	0.66
1:B:222:PHE:CZ	1:B:226:ILE:HD11	2.32	0.64
1:B:191:ASP:CG	1:B:195:ARG:HE	2.01	0.64
2:D:66:G:H2'	2:D:67:C:C6	2.33	0.64
1:B:23:ILE:HG13	1:B:156:PHE:HB3	1.78	0.64
2:D:33:U:O4	2:D:36:A:N1	2.30	0.64
1:A:79:TYR:CE2	2:C:74:C:H5'	2.33	0.63
1:A:116:ARG:NH2	3:A:2001:ANP:C5'	2.61	0.63
1:A:194:THR:O	1:A:198:VAL:HG23	1.98	0.63
1:B:192:LYS:CE	2:D:16:U:H5'	2.25	0.62
1:A:79:TYR:HE2	2:C:74:C:H5'	1.64	0.62
2:D:38:A:O2'	2:D:39:U:H5'	2.00	0.62
2:D:47:G:H2'	2:D:47(A):C:C6	2.34	0.61
1:B:108:VAL:O	1:B:112:ARG:HG3	2.01	0.61
2:C:70:G:H2'	2:C:71:C:C6	2.35	0.61
2:D:66:G:H2'	2:D:67:C:H6	1.65	0.61
1:B:207:LEU:HD22	1:B:211:LYS:HD3	1.83	0.61
1:A:23:ILE:HG13	1:A:156:PHE:HB3	1.80	0.61
1:B:197:ILE:HG22	1:B:245:LEU:CD1	2.32	0.60
1:B:149:ASP:OD2	1:B:152:LYS:HG3	2.02	0.60
1:B:213:LYS:O	1:B:217:GLU:HG2	2.01	0.60
1:B:233:ASP:HB3	1:B:236:ARG:HG3	1.84	0.60
2:D:15:G:H2'	2:D:16:U:C6	2.38	0.59
2:D:39:U:H2'	2:D:40:C:C6	2.37	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:210:ASP:O	1:B:214:GLU:HG3	2.02	0.59
1:A:102:LEU:CD2	1:A:148:ILE:HB	2.32	0.59
1:B:226:ILE:HD13	1:B:237:VAL:CG1	2.32	0.59
1:B:93:TYR:O	1:B:95:LYS:HE2	2.03	0.58
1:B:222:PHE:CE2	1:B:226:ILE:HD11	2.39	0.57
2:D:29:G:H2'	2:D:30:G:H8	1.68	0.57
1:A:145:PHE:CD2	1:A:146:LEU:HG	2.40	0.57
1:A:176:LEU:HD12	1:A:177:GLU:H	1.70	0.57
2:C:32:C:N4	2:C:37:G:N7	2.53	0.56
1:B:197:ILE:HG22	1:B:245:LEU:HD11	1.87	0.56
1:A:175:VAL:CG1	1:A:176:LEU:H	2.17	0.56
1:B:22:LYS:O	1:B:25:SER:HB3	2.06	0.56
2:C:52:G:O2'	2:C:53:G:H5'	2.06	0.56
2:D:45:G:O2'	2:D:46:C:H5'	2.06	0.56
1:A:55:LYS:HE2	1:A:59:TYR:HE2	1.70	0.56
2:D:47(N):G:O2'	2:D:48:C:H5'	2.06	0.56
1:B:199:SER:HA	2:D:19:G:O6	2.06	0.55
2:C:68:C:H2'	2:C:69:G:O4'	2.06	0.55
2:D:59:U:C2'	2:D:60:U:H5'	2.37	0.55
1:B:92:LYS:HE2	1:B:93:TYR:CZ	2.42	0.55
1:B:18:LYS:O	1:B:22:LYS:HG3	2.07	0.54
1:B:189:LYS:O	1:B:193:GLU:HG2	2.08	0.54
2:D:19:G:H1'	2:D:20:U:OP2	2.08	0.54
1:B:222:PHE:CE2	1:B:241:PHE:HB2	2.43	0.54
1:B:232:VAL:HG13	1:B:237:VAL:CG2	2.37	0.54
2:C:70:G:H2'	2:C:71:C:H6	1.73	0.54
1:B:67:LYS:HG2	1:B:93:TYR:CE1	2.42	0.53
1:B:171:PRO:HB2	1:B:173:PHE:CE1	2.44	0.53
1:B:171:PRO:HB2	1:B:173:PHE:HE1	1.74	0.53
2:D:23:C:H2'	2:D:24:G:C8	2.41	0.53
1:B:105:SER:OG	1:B:108:VAL:HG23	2.08	0.53
1:A:229:MSE:HE3	1:A:232:VAL:HG22	1.91	0.53
1:A:242:LYS:O	1:A:246:ASN:ND2	2.42	0.53
1:B:1:MSE:HB2	1:B:96:ASN:O	2.08	0.53
1:B:207:LEU:HD13	1:B:211:LYS:HB3	1.90	0.53
2:D:14:G:O2'	2:D:15:G:H5'	2.09	0.53
2:D:37:G:C2'	2:D:38:A:H5'	2.39	0.53
1:B:234:ALA:O	1:B:238:LEU:HG	2.09	0.53
1:B:155:ASP:OD2	1:B:158:GLU:HB2	2.09	0.53
2:C:38:A:O5'	2:C:38:A:C8	2.61	0.53
1:B:78:TYR:HE2	1:B:82:MSE:HE1	1.72	0.53
2:D:21:C:H2'	2:D:22:C:H6	1.74	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:PHE:CE1	1:A:148:ILE:HD13	2.44	0.52
1:B:166:LYS:HA	1:B:169:GLU:HG3	1.90	0.52
1:A:19:ASN:O	1:A:23:ILE:HG12	2.09	0.52
1:B:201:TYR:CD2	1:B:245:LEU:HD22	2.43	0.52
1:A:13:LYS:NZ	3:A:2001:ANP:O1B	2.39	0.52
1:A:202:ILE:CD1	1:A:212:ILE:HG23	2.39	0.52
1:A:202:ILE:HD13	1:A:212:ILE:HG23	1.92	0.52
2:C:15:G:O2'	2:C:16:U:H5'	2.10	0.52
1:A:1:MSE:HB2	1:A:96:ASN:O	2.10	0.51
1:B:79:TYR:HB2	1:B:82:MSE:HG3	1.92	0.51
1:B:0:HIS:HB2	1:B:70:TRP:CD1	2.45	0.51
1:B:112:ARG:O	1:B:116:ARG:HG2	2.10	0.51
2:C:53:G:H2'	2:C:54:U:H6	1.76	0.51
1:B:110:ILE:O	1:B:114:ILE:HG13	2.10	0.51
1:B:123:GLU:O	1:B:127:LYS:HD3	2.11	0.51
1:A:160:ALA:O	1:A:164:ILE:HG13	2.11	0.51
1:A:176:LEU:HG	1:A:177:GLU:N	2.26	0.51
1:A:67:LYS:HE2	1:A:93:TYR:OH	2.11	0.51
1:A:55:LYS:HE2	1:A:59:TYR:CE2	2.46	0.51
2:C:37:G:C2'	2:C:38:A:C8	2.93	0.50
1:A:95:LYS:O	1:A:173:PHE:HZ	1.94	0.50
1:A:198:VAL:HG13	1:A:215:VAL:HG12	1.93	0.50
2:D:29:G:H2'	2:D:30:G:C8	2.44	0.50
2:D:40:C:H2'	2:D:41:C:C6	2.47	0.50
1:B:220:LYS:HG2	1:B:224:LYS:HE3	1.93	0.50
1:A:108:VAL:O	1:A:112:ARG:HG3	2.11	0.50
1:A:18:LYS:O	1:A:22:LYS:HG3	2.12	0.49
1:B:123:GLU:HG3	1:B:124:VAL:N	2.27	0.49
1:A:175:VAL:HG13	1:A:176:LEU:H	1.76	0.49
1:A:232:VAL:HG13	1:A:237:VAL:CG2	2.41	0.49
1:B:233:ASP:OD2	1:B:236:ARG:HG3	2.12	0.49
1:A:158:GLU:HG3	1:A:162:LYS:HE3	1.94	0.49
2:D:47(E):G:C2'	2:D:47(G):G:H5''	2.38	0.49
2:D:1:G:H2'	2:D:2:G:H8	1.78	0.49
1:B:198:VAL:O	1:B:202:ILE:HG13	2.13	0.49
1:A:178:GLU:O	1:A:179:ASN:HB2	2.12	0.49
1:A:92:LYS:HE2	1:A:93:TYR:CZ	2.47	0.49
1:A:193:GLU:O	1:A:197:ILE:HG13	2.13	0.49
2:D:47(E):G:OP1	2:D:47(F):A:H5'	2.13	0.49
1:B:20:LEU:HD12	1:B:20:LEU:O	2.13	0.49
2:C:4:C:H2'	2:C:5:G:H8	1.78	0.48
2:C:30:G:O2'	2:C:31:A:H5'	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:37:G:C8	2:C:37:G:OP1	2.66	0.48
1:A:215:VAL:HG13	1:A:245:LEU:HD21	1.95	0.48
2:D:37:G:H2'	2:D:38:A:H5'	1.94	0.48
1:B:211:LYS:HA	1:B:214:GLU:OE1	2.14	0.48
1:A:198:VAL:O	1:A:202:ILE:HG13	2.13	0.47
2:D:1:G:H2'	2:D:2:G:C8	2.48	0.47
2:C:59:U:C2'	2:C:60:U:H5'	2.44	0.47
2:D:66:G:O2'	2:D:67:C:H5'	2.13	0.47
1:A:110:ILE:O	1:A:114:ILE:HG13	2.15	0.47
1:B:199:SER:O	1:B:203:LYS:HG3	2.15	0.47
2:D:18:G:H4'	2:D:60:U:C2	2.49	0.47
2:D:47(N):G:C2'	2:D:48:C:H5'	2.44	0.47
2:D:21:C:O2'	2:D:22:C:H5'	2.15	0.47
2:C:47(H):U:H2'	2:C:47(I):G:O4'	2.14	0.47
1:A:111:ARG:HG3	1:A:111:ARG:HH11	1.80	0.47
1:A:232:VAL:HG13	1:A:237:VAL:HG21	1.96	0.47
2:C:11:C:O2'	2:C:12:G:H5'	2.14	0.47
2:C:20:U:OP1	2:C:20:U:H3'	2.14	0.47
1:B:191:ASP:OD2	1:B:195:ARG:NE	2.47	0.47
2:D:21:C:H2'	2:D:22:C:C6	2.49	0.47
1:B:190:ILE:O	1:B:194:THR:HG23	2.15	0.47
1:A:208:ASP:O	1:A:212:ILE:HG13	2.16	0.46
1:B:145:PHE:CD2	1:B:146:LEU:HG	2.50	0.46
1:A:188:ASP:OD2	1:A:192:LYS:HE3	2.14	0.46
1:B:118:GLU:CD	1:B:122:ASN:ND2	2.68	0.46
2:D:42:G:O2'	2:D:43:G:H5'	2.15	0.46
1:A:10:GLY:HA2	1:A:116:ARG:NH2	2.30	0.46
1:B:232:VAL:CG1	1:B:237:VAL:HG21	2.44	0.46
2:D:42:G:H2'	2:D:43:G:O4'	2.16	0.46
1:A:102:LEU:HD22	1:A:148:ILE:HB	1.97	0.45
2:D:36:A:H2'	2:D:37:G:H8	1.77	0.45
2:D:45:G:H2'	2:D:46:C:H6	1.81	0.45
2:D:70:G:H2'	2:D:71:C:C6	2.52	0.45
2:C:28:C:H2'	2:C:29:G:H8	1.82	0.45
2:D:14:G:H2'	2:D:15:G:H8	1.81	0.45
1:B:216:VAL:HG13	2:D:20:U:OP2	2.17	0.45
1:B:40:ARG:HB2	1:B:54:ILE:HD13	1.99	0.45
2:D:47(K):G:H2'	2:D:47(L):G:H8	1.82	0.44
1:B:0:HIS:CB	1:B:70:TRP:CD1	3.00	0.44
1:B:1:MSE:HG2	1:B:70:TRP:CZ3	2.53	0.44
2:D:40:C:H2'	2:D:41:C:H6	1.81	0.44
2:D:54:U:H2'	2:D:55:U:H5'	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:0:HIS:HA	1:A:70:TRP:NE1	2.33	0.44
2:C:32:C:N4	2:C:37:G:C8	2.86	0.44
2:D:38:A:H2'	2:D:39:U:H6	1.82	0.44
1:A:198:VAL:HG13	1:A:215:VAL:CG1	2.46	0.44
2:D:2:G:H2'	2:D:3:C:C6	2.53	0.44
2:C:39:U:H2'	2:C:40:C:C6	2.52	0.44
2:C:28:C:H2'	2:C:29:G:C8	2.53	0.44
2:D:47(C):C:H2'	2:D:47(D):C:H6	1.77	0.43
2:D:36:A:H2'	2:D:37:G:N7	2.33	0.43
2:D:37:G:O2'	2:D:38:A:H5'	2.18	0.43
1:B:84:ARG:HB2	1:B:141:TRP:CH2	2.53	0.43
1:A:24:LEU:O	1:A:29:ILE:HB	2.18	0.43
1:B:207:LEU:HB3	1:B:211:LYS:HB2	2.00	0.43
1:B:-1:HIS:HB3	1:B:0:HIS:H	1.68	0.43
2:C:53:G:H2'	2:C:54:U:C6	2.52	0.43
2:C:24:G:O2'	2:C:25:G:H5'	2.19	0.43
1:A:176:LEU:CG	1:A:177:GLU:N	2.82	0.43
2:D:9:A:H1'	2:D:45:G:C6	2.53	0.43
2:D:18:G:H1	2:D:55:U:H1'	1.84	0.43
1:A:232:VAL:CG1	1:A:237:VAL:HG21	2.49	0.43
2:D:2:G:H2'	2:D:3:C:H6	1.84	0.43
1:A:50:TYR:O	1:A:54:ILE:HG13	2.19	0.43
1:B:198:VAL:HG21	1:B:219:ARG:HD3	2.01	0.43
2:D:35:C:O2'	2:D:36:A:P	2.77	0.43
1:A:176:LEU:CD1	1:A:177:GLU:H	2.31	0.43
2:D:9:A:H1'	2:D:45:G:C5	2.54	0.43
1:B:185:ASN:O	1:B:189:LYS:HG3	2.19	0.43
1:B:0:HIS:HA	1:B:70:TRP:CD1	2.54	0.42
2:D:59:U:H2'	2:D:60:U:O4'	2.19	0.42
1:B:197:ILE:HG22	1:B:245:LEU:HD12	2.00	0.42
1:B:197:ILE:CG2	1:B:245:LEU:HD12	2.49	0.42
1:A:8:LEU:CD1	1:A:129:TYR:HA	2.45	0.42
1:B:149:ASP:OD2	1:B:151:THR:OG1	2.38	0.42
1:B:38:LEU:HD23	1:B:38:LEU:HA	1.71	0.42
2:C:29:G:H2'	2:C:30:G:C8	2.55	0.42
1:B:194:THR:O	1:B:198:VAL:HG23	2.19	0.42
1:A:192:LYS:O	1:A:195:ARG:HB3	2.20	0.42
2:C:40:C:O2'	2:C:41:C:H5'	2.20	0.42
1:A:102:LEU:HD23	1:A:148:ILE:HB	2.01	0.41
1:B:145:PHE:CE1	1:B:166:LYS:HD2	2.55	0.41
1:A:76:THR:HG22	1:A:78:TYR:HB3	2.02	0.41
1:B:47:LYS:HD2	1:B:50:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:37:ASP:O	1:A:38:LEU:C	2.57	0.41
1:A:140:LYS:HD2	2:C:68:C:OP1	2.21	0.41
1:B:91:LYS:HA	1:B:173:PHE:CE2	2.55	0.41
2:C:75:C:OP1	2:C:76:A:O3'	2.34	0.41
1:A:78:TYR:HB2	1:A:132:PHE:CD1	2.44	0.41
1:A:226:ILE:HD13	1:A:237:VAL:CG1	2.51	0.41
1:A:116:ARG:NH2	3:A:2001:ANP:HNB1	2.01	0.41
2:C:42:G:H2'	2:C:43:G:O4'	2.21	0.41
1:B:220:LYS:O	1:B:224:LYS:HG3	2.21	0.41
1:B:0:HIS:HA	1:B:70:TRP:HE1	1.81	0.41
1:A:16:PHE:HE1	1:A:148:ILE:HD13	1.86	0.41
2:D:47(K):G:O2'	2:D:47(L):G:H5'	2.21	0.41
2:D:47(I):G:H2'	2:D:47(J):G:O4'	2.21	0.41
1:B:121:PRO:HG2	1:B:124:VAL:HG21	1.99	0.40
1:B:118:GLU:OE1	1:B:122:ASN:ND2	2.52	0.40
1:B:24:LEU:O	1:B:29:ILE:HB	2.21	0.40
2:D:26:G:H2'	2:D:27:C:O4'	2.21	0.40
1:B:215:VAL:O	1:B:218:LEU:HB3	2.22	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	242/259 (93%)	234 (97%)	8 (3%)	0	100	100
1	B	235/259 (91%)	225 (96%)	10 (4%)	0	100	100
All	All	477/518 (92%)	459 (96%)	18 (4%)	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	233/241 (97%)	232 (100%)	1 (0%)	95	99
1	B	226/241 (94%)	224 (99%)	2 (1%)	87	97
All	All	459/482 (95%)	456 (99%)	3 (1%)	91	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
1	B	75	ASP
1	B	78	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	28	ASN
1	A	246	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	86/92 (93%)	7 (8%)	2 (2%)
2	D	91/92 (98%)	14 (15%)	2 (2%)
All	All	177/184 (96%)	21 (11%)	4 (2%)

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	8	C
2	C	18	G
2	C	20	U
2	C	20(A)	C
2	C	32	C

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Mol	Chain	Res	Type
2	C	39	U
2	C	74	C
2	D	8	C
2	D	9	A
2	D	18	G
2	D	20	U
2	D	20(A)	C
2	D	32	C
2	D	33	U
2	D	34	U
2	D	36	A
2	D	37	G
2	D	47(G)	G
2	D	47(I)	G
2	D	61	C
2	D	76	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	19	G
2	C	38	A
2	D	19	G
2	D	35	C

## 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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ANP	A	2001	4	33,33,33	1.71	8 (24%)	51,52,52	2.03	10 (19%)
3	ANP	B	2002	4	33,33,33	1.76	8 (24%)	51,52,52	2.11	12 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	2001	4	-	0/18/38/38	0/1/3/3
3	ANP	B	2002	4	-	0/18/38/38	0/1/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	ANP	PG-N3B	-3.85	1.61	1.64
3	A	2001	ANP	O4'-C1'	3.58	1.46	1.41
3	B	2002	ANP	PA-O3A	3.51	1.66	1.59
3	B	2002	ANP	PG-N3B	-3.45	1.61	1.64
3	B	2002	ANP	PB-O3A	3.30	1.63	1.59
3	B	2002	ANP	O4'-C1'	3.24	1.46	1.41
3	A	2001	ANP	PB-O3A	3.14	1.63	1.59
3	A	2001	ANP	PA-O3A	3.11	1.65	1.59
3	B	2002	ANP	C4-N9	-2.90	1.33	1.37
3	B	2002	ANP	PG-O1G	2.88	1.49	1.46
3	A	2001	ANP	PG-O1G	2.83	1.49	1.46
3	B	2002	ANP	PG-O2G	2.75	1.63	1.55
3	A	2001	ANP	PB-O1B	2.74	1.49	1.46
3	A	2001	ANP	PG-O2G	2.73	1.63	1.55
3	A	2001	ANP	C4-N9	-2.61	1.33	1.37
3	B	2002	ANP	PB-O1B	2.54	1.49	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	ANP	N3-C2-N1	-8.98	121.20	128.71
3	A	2001	ANP	N3-C2-N1	-8.92	121.25	128.71
3	B	2002	ANP	PB-N3B-PG	-4.94	121.76	130.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	ANP	N3-C4-N9	4.39	133.37	125.43
3	A	2001	ANP	O2B-PB-O1B	4.31	119.83	109.89
3	A	2001	ANP	PB-N3B-PG	-4.28	122.87	130.07
3	A	2001	ANP	N3-C4-N9	4.27	133.14	125.43
3	B	2002	ANP	O2B-PB-O1B	4.12	119.41	109.89
3	B	2002	ANP	PA-O3A-PB	-3.04	121.43	131.81
3	B	2002	ANP	C4'-O4'-C1'	-3.00	106.49	109.75
3	A	2001	ANP	C4'-O4'-C1'	-2.99	106.50	109.75
3	B	2002	ANP	C5-C4-N3	-2.86	119.46	125.70
3	A	2001	ANP	C5-C4-N3	-2.82	119.55	125.70
3	A	2001	ANP	PA-O3A-PB	-2.60	122.93	131.81
3	B	2002	ANP	O4'-C1'-N9	2.58	110.84	108.44
3	B	2002	ANP	C2-N3-C4	2.30	120.55	114.01
3	B	2002	ANP	O1B-PB-N3B	-2.27	108.39	111.83
3	A	2001	ANP	C2-N3-C4	2.27	120.47	114.01
3	A	2001	ANP	C4-C5-N7	-2.17	107.66	109.52
3	A	2001	ANP	O1B-PB-N3B	-2.09	108.66	111.83
3	B	2002	ANP	O4'-C1'-C2'	-2.09	103.57	106.77
3	B	2002	ANP	C4-C5-N7	-2.02	107.79	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	246/259 (94%)	0.37	16 (6%) 18 22	60, 90, 153, 200	0
1	B	239/259 (92%)	0.43	18 (7%) 14 17	61, 101, 178, 196	0
2	C	88/92 (95%)	0.23	2 (2%) 57 66	58, 87, 141, 197	0
2	D	92/92 (100%)	1.08	17 (18%) 2 3	72, 148, 201, 201	0
All	All	665/702 (94%)	0.47	53 (7%) 13 15	58, 97, 184, 201	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	34	U	8.5
2	D	47(F)	A	7.8
1	A	231	GLU	7.0
1	B	227	LYS	6.6
1	B	209	LYS	6.5
1	A	178	GLU	6.1
1	A	174	TYR	5.3
2	D	30	G	5.3
2	D	32	C	5.2
2	D	35	C	5.2
1	A	116	ARG	4.6
2	D	47(G)	G	4.4
2	D	29	G	4.4
2	D	36	A	4.3
1	A	179	ASN	4.0
1	A	117	GLY	4.0
1	B	248	TYR	3.8
1	B	210	ASP	3.6
1	B	206	LYS	3.5
1	A	232	VAL	3.5
1	B	-1	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	33	U	3.4
1	B	228	LYS	3.3
2	C	32	C	3.3
2	D	37	G	3.3
1	B	229	MSE	3.2
2	D	31	A	3.2
2	C	37	G	3.1
2	D	47(H)	U	3.1
1	A	230	GLU	3.0
2	D	38	A	2.8
1	A	78	TYR	2.7
1	B	236	ARG	2.6
1	B	231	GLU	2.6
1	B	226	ILE	2.6
1	B	246	ASN	2.6
1	B	223	LEU	2.4
1	A	126	LYS	2.4
2	D	58	A	2.4
1	A	45	VAL	2.3
1	A	236	ARG	2.2
2	D	8	C	2.2
1	B	225	LYS	2.2
1	B	230	GLU	2.2
1	A	79	TYR	2.2
1	B	208	ASP	2.1
1	B	189	LYS	2.1
1	A	3	ILE	2.1
1	A	202	ILE	2.1
2	D	47(D)	C	2.1
1	A	137	LYS	2.0
2	D	51	G	2.0
1	B	204	SER	2.0

## 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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ANP	A	2001	31/31	0.23	-	99,148,165,166	0
3	ANP	B	2002	31/31	0.18	-	86,119,128,135	0
4	MG	A	2003	1/1	0.09	-	93,93,93,93	0
4	MG	B	2004	1/1	0.07	-	77,77,77,77	0

## 6.5 Other polymers

There are no such residues in this entry.