



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:28 pm GMT

PDB ID : 3ADD  
Title : Crystal structure of O-phosphoseryl-tRNA kinase complexed with selenocysteine tRNA and AMPPNP (crystal type 3)  
Authors : Itoh, Y.; Chiba, S.; Sekine, S.; Yokoyama, S.  
Deposited on : 2010-01-18  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

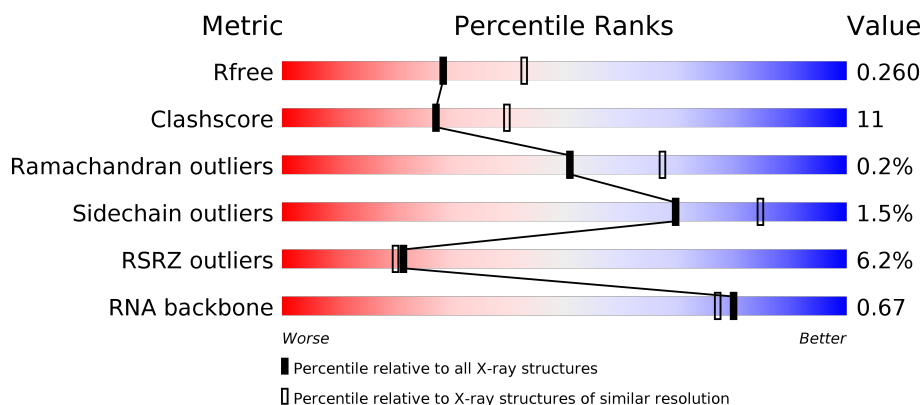
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)
RNA backbone	2435	1034 (2.86-1.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	259	<div> <div>4%</div> <div>75%</div> <div>21%</div> <div>••</div> </div>
1	B	259	<div> <div>8%</div> <div>65%</div> <div>26%</div> <div>• 8%</div> </div>
2	C	92	<div> <div>5%</div> <div>53%</div> <div>35%</div> <div>7% ••</div> </div>
2	D	92	<div> <div>7%</div> <div>39%</div> <div>50%</div> <div>7% •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ANP	A	2001	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8109 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 L-seryl-tRNA(Sec) kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	Se	0	0	0
			2109	1365	352	388	4			
1	B	239	Total	C	N	O	Se	0	0	0
			2004	1301	332	367	4			

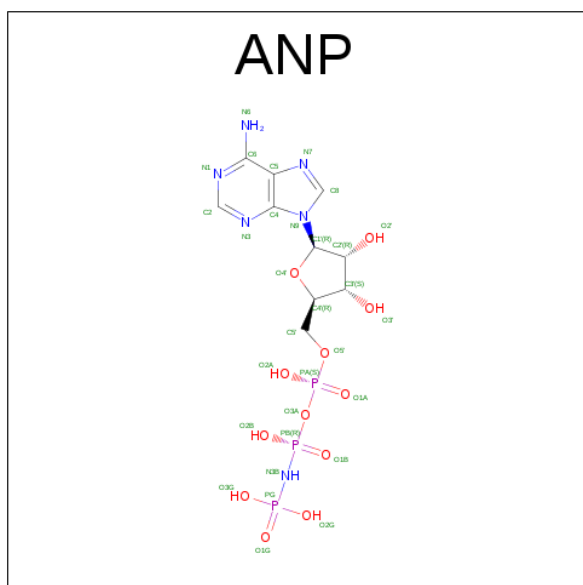
There are 22 discrepancies between the modelled and reference sequences:

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	88	Total	C	N	O	P	0	0	0
			1886	836	343	619	88			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-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	46	Total	O	0	0
			46	46		

*Continued on next page...*

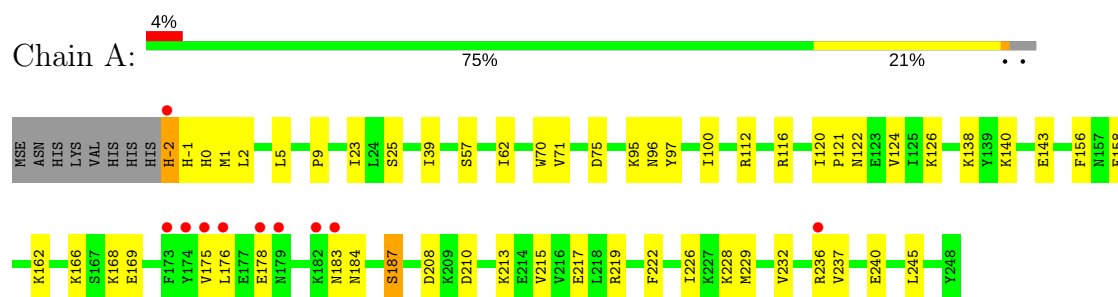
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	47	Total 47	O 47	0	0
5	C	49	Total 49	O 49	0	0
5	D	18	Total 18	O 18	0	0

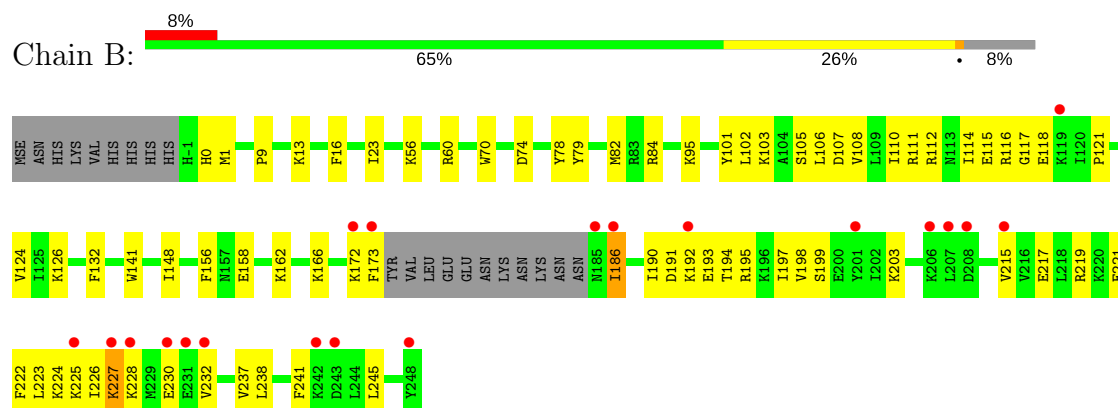
### 3 Residue-property plots

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.

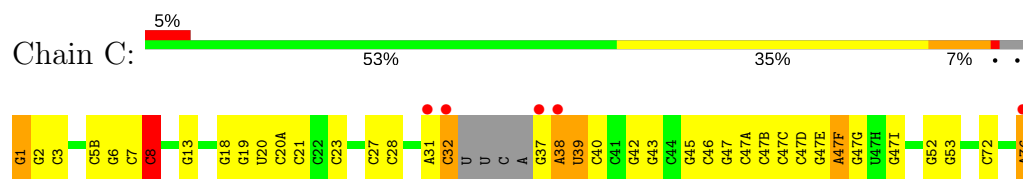
- Molecule 1: L-seryl-tRNA(Sec) kinase



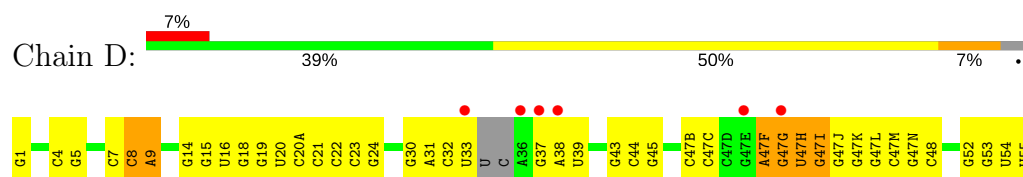
- Molecule 1: L-seryl-tRNA(Sec) kinase



- Molecule 2: selenocysteine tRNA



- Molecule 2: selenocysteine tRNA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.86Å 258.90Å 45.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.55 – 2.40 40.55 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.1 (40.55-2.40) 91.2 (40.55-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.218 , 0.258 0.219 , 0.260	Depositor DCC
$R_{free}$ test set	2035 reflections (5.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.8	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 47.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: 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	0.47	0/2141	0.66	0/2858
1	B	0.48	0/2033	0.68	0/2711
2	C	0.54	1/2104 (0.0%)	0.77	2/3278 (0.1%)
2	D	0.48	1/2104 (0.0%)	0.75	1/3278 (0.0%)
All	All	0.49	2/8382 (0.0%)	0.72	3/12125 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	G	OP3-P	-6.94	1.52	1.61
2	D	1	G	OP3-P	-6.17	1.53	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8	C	C5'-C4'-C3'	-6.17	106.13	116.00
2	C	19	G	C2'-C3'-O3'	6.04	123.36	113.70
2	D	19	G	C2'-C3'-O3'	5.00	121.70	113.70

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	2109	0	2211	47	0
1	B	2004	0	2112	54	0
2	C	1886	0	962	29	0
2	D	1886	0	961	37	0
3	A	31	0	13	9	0
3	B	31	0	13	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	46	0	0	1	0
5	B	47	0	0	0	0
5	C	49	0	0	0	0
5	D	18	0	0	1	0
All	All	8109	0	6272	162	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 11.

All (162) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:C:H5''	2:D:8:C:H5'	1.40	1.03
1:A:-2:HIS:HB2	1:A:168:LYS:HG2	1.42	0.99
2:C:7:C:H5''	2:C:8:C:H5'	1.46	0.95
1:A:116:ARG:HH22	3:A:2001:ANP:HNB1	1.09	0.90
1:A:116:ARG:HH21	3:A:2001:ANP:H5'2	1.38	0.89
1:B:219:ARG:NH1	1:B:223:LEU:HD11	1.94	0.82
1:B:191:ASP:O	1:B:195:ARG:HG3	1.81	0.80
1:B:0:HIS:HB2	1:B:70:TRP:CD1	2.18	0.78
1:A:-1:HIS:NE2	1:A:95:LYS:NZ	2.33	0.75
1:A:62:ILE:HG23	1:A:71:VAL:HG11	1.68	0.75
1:A:116:ARG:HH21	3:A:2001:ANP:C5'	2.00	0.74
1:A:1:MSE:HE3	1:A:96:ASN:HB3	1.69	0.74
2:D:32:C:O2	2:D:38:A:N1	2.22	0.72
1:B:221:GLU:HG2	1:B:225:LYS:HE3	1.72	0.72
2:D:47(G):G:C6	2:D:47(I):G:H1'	2.24	0.72
2:D:47(F):A:O2'	2:D:47(G):G:C5'	2.38	0.71
1:B:1:MSE:HE1	1:B:166:LYS:HG2	1.73	0.71
1:B:222:PHE:CZ	1:B:226:ILE:HD11	2.27	0.69
2:C:47(C):C:H2'	2:C:47(D):C:C6	2.28	0.69
1:B:56:LYS:HE2	1:B:60:ARG:HH21	1.57	0.68
1:A:116:ARG:NH2	3:A:2001:ANP:HNB1	1.89	0.67
2:D:38:A:H2'	2:D:39:U:C6	2.30	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLU:OE1	1:B:238:LEU:HD11	1.94	0.66
1:B:186:ILE:O	1:B:190:ILE:HG13	1.96	0.66
1:B:23:ILE:HG13	1:B:156:PHE:HB3	1.78	0.65
1:B:0:HIS:HE2	1:B:95:LYS:HE3	1.62	0.65
1:B:0:HIS:NE2	1:B:95:LYS:HE3	2.11	0.65
2:D:47(L):G:H2'	2:D:47(M):C:C6	2.32	0.65
1:B:198:VAL:HG21	1:B:219:ARG:HD3	1.79	0.65
2:C:47:G:H2'	2:C:47(A):C:C6	2.32	0.64
2:D:23:C:H2'	2:D:24:G:H8	1.64	0.63
1:B:102:LEU:HD23	1:B:148:ILE:HB	1.81	0.62
1:A:0:HIS:HB2	1:A:70:TRP:CD1	2.34	0.62
1:A:121:PRO:HG2	1:A:124:VAL:CG2	2.29	0.61
1:B:224:LYS:HA	1:B:227:LYS:HE3	1.82	0.61
2:C:39:U:H2'	2:C:40:C:C6	2.36	0.61
1:B:192:LYS:HE2	2:D:15:G:O2'	2.01	0.60
1:B:108:VAL:HA	1:B:111:ARG:HD2	1.83	0.60
1:B:56:LYS:CE	1:B:60:ARG:HH21	2.14	0.60
1:A:208:ASP:OD1	1:A:210:ASP:HB2	2.02	0.60
1:B:0:HIS:CB	1:B:70:TRP:CD1	2.84	0.60
1:A:0:HIS:NE2	1:A:95:LYS:HE3	2.18	0.59
2:D:23:C:H2'	2:D:24:G:C8	2.38	0.59
1:B:16:PHE:CE1	1:B:148:ILE:HD13	2.38	0.59
2:C:32:C:O2	2:C:38:A:N6	2.36	0.59
1:B:232:VAL:HG13	1:B:237:VAL:HG21	1.85	0.59
2:D:47(F):A:HO2'	2:D:47(G):G:C5'	2.16	0.59
1:A:121:PRO:HG2	1:A:124:VAL:HG23	1.85	0.57
1:B:226:ILE:HD13	1:B:237:VAL:CG1	2.34	0.57
1:B:106:LEU:HD21	1:B:126:LYS:HG2	1.86	0.56
1:B:158:GLU:OE2	1:B:162:LYS:HE3	2.04	0.56
2:D:47(F):A:O2'	2:D:47(G):G:H5'	2.04	0.56
2:C:47(D):C:H2'	2:C:47(E):G:O4'	2.06	0.56
1:A:226:ILE:CD1	1:A:237:VAL:HG13	2.36	0.56
2:D:52:G:O2'	2:D:53:G:H5'	2.05	0.56
1:A:219:ARG:NH2	2:C:21:C:O2'	2.39	0.56
1:A:23:ILE:HG13	1:A:156:PHE:HB3	1.88	0.56
2:D:37:G:H2'	2:D:38:A:N9	2.20	0.56
1:A:116:ARG:NH2	3:A:2001:ANP:C5'	2.67	0.55
1:A:222:PHE:CE2	1:A:226:ILE:HD12	2.41	0.55
2:D:9:A:H1'	2:D:45:G:C5	2.42	0.55
2:D:59:U:O2'	2:D:60:U:H5'	2.05	0.55
2:C:31:A:H2'	2:C:32:C:C4'	2.37	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:47(C):C:H2'	2:C:47(D):C:H6	1.71	0.55
2:D:4:C:H2'	2:D:5:G:O4'	2.07	0.55
2:C:39:U:H2'	2:C:40:C:H6	1.71	0.55
2:D:30:G:O2'	2:D:31:A:H5'	2.07	0.55
2:D:15:G:O2'	2:D:16:U:H5'	2.06	0.54
1:B:116:ARG:NH1	3:B:2002:ANP:H5'2	2.22	0.54
2:D:47(H):U:O2'	2:D:47(I):G:P	2.65	0.54
1:B:222:PHE:CE2	1:B:241:PHE:HB2	2.42	0.54
1:A:0:HIS:CB	1:A:70:TRP:CD1	2.90	0.54
2:C:31:A:H3'	2:C:32:C:H5''	1.89	0.54
1:B:116:ARG:HH22	3:B:2002:ANP:HNB1	1.55	0.53
2:C:31:A:H2'	2:C:32:C:H4'	1.90	0.53
1:B:111:ARG:O	1:B:115:GLU:HG3	2.09	0.53
1:B:112:ARG:O	1:B:116:ARG:HG3	2.09	0.53
1:A:138:LYS:HE2	2:C:1:G:OP2	2.09	0.52
1:B:13:LYS:HB3	1:B:74:ASP:OD1	2.09	0.52
1:B:0:HIS:HB2	1:B:70:TRP:HD1	1.74	0.52
2:D:47(H):U:O2'	2:D:47(I):G:OP1	2.27	0.52
1:A:236:ARG:O	1:A:240:GLU:HG3	2.10	0.52
1:A:0:HIS:HA	1:A:70:TRP:NE1	2.25	0.51
3:A:2001:ANP:H2'	3:A:2001:ANP:O5'	2.10	0.51
1:A:-1:HIS:CG	1:A:0:HIS:H	2.29	0.51
2:C:38:A:OP2	2:C:38:A:H8	1.92	0.51
2:C:52:G:O2'	2:C:53:G:H5'	2.11	0.50
2:D:47(L):G:H2'	2:D:47(M):C:H6	1.75	0.50
1:B:121:PRO:HG2	1:B:124:VAL:CG2	2.41	0.50
1:B:79:TYR:HB2	1:B:82:MSE:HG3	1.94	0.50
1:B:197:ILE:HD12	1:B:241:PHE:HD2	1.77	0.50
2:C:47(E):G:C2'	2:C:47(F):A:H5'	2.41	0.50
2:D:70:G:H2'	2:D:71:C:C6	2.45	0.50
2:D:62:C:H2'	2:D:63:C:H6	1.77	0.50
1:B:199:SER:O	1:B:203:LYS:HG3	2.12	0.49
1:A:112:ARG:HD3	3:A:2001:ANP:O4'	2.13	0.49
1:A:120:ILE:HG12	2:C:76:A:C2	2.48	0.48
1:A:184:ASN:OD1	1:A:187:SER:HB2	2.12	0.48
1:A:122:ASN:O	1:A:126:LYS:HG3	2.14	0.48
1:B:215:VAL:HG13	1:B:245:LEU:HD21	1.96	0.48
2:D:21:C:H2'	2:D:22:C:C6	2.49	0.47
2:D:57:A:H2'	2:D:58:A:H5'	1.96	0.47
1:B:193:GLU:CD	1:B:238:LEU:HD11	2.35	0.47
2:D:43:G:O2'	2:D:44:C:H5'	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:HG13	1:A:245:LEU:HD21	1.97	0.47
1:A:213:LYS:O	1:A:217:GLU:HG3	2.15	0.47
1:A:166:LYS:HA	1:A:169:GLU:OE2	2.14	0.47
2:C:38:A:OP2	2:C:38:A:C8	2.68	0.47
2:D:47(K):G:O2'	2:D:47(L):G:H5'	2.15	0.47
2:D:21:C:H2'	2:D:22:C:H6	1.80	0.46
1:A:183:ASN:HD21	2:C:23:C:C4'	2.28	0.46
2:D:54:U:H2'	2:D:55:U:H5'	1.98	0.46
1:B:106:LEU:O	1:B:110:ILE:HG12	2.15	0.46
1:A:116:ARG:NH2	3:A:2001:ANP:H5'1	2.31	0.46
2:C:42:G:H2'	2:C:43:G:O4'	2.16	0.45
1:A:5:LEU:HD23	1:A:100:ILE:HB	1.97	0.45
1:B:225:LYS:O	1:B:228:LYS:HB2	2.16	0.45
2:C:45:G:H2'	2:C:46:C:C6	2.51	0.45
2:C:2:G:H2'	2:C:3:C:C6	2.52	0.45
2:C:47(B):C:O2'	2:C:47(C):C:H5'	2.17	0.45
2:D:38:A:H2'	2:D:39:U:O4'	2.15	0.45
1:A:176:LEU:HD23	2:C:13:G:OP1	2.17	0.45
1:B:219:ARG:O	1:B:223:LEU:HG	2.17	0.45
1:B:107:ASP:O	1:B:111:ARG:HG3	2.17	0.45
1:B:105:SER:OG	1:B:108:VAL:HG23	2.16	0.45
1:A:39:ILE:CD1	1:A:57:SER:HB3	2.47	0.44
2:D:62:C:H2'	2:D:63:C:C6	2.53	0.44
1:B:226:ILE:HD13	1:B:237:VAL:HG13	1.98	0.44
1:A:140:LYS:HA	1:A:143:GLU:OE2	2.18	0.44
1:B:9:PRO:HA	3:B:2002:ANP:O2G	2.18	0.43
1:B:110:ILE:O	1:B:114:ILE:HG13	2.19	0.43
1:A:175:VAL:HG13	1:A:178:GLU:OE1	2.19	0.43
1:A:232:VAL:HG13	1:A:237:VAL:HG21	1.99	0.43
1:B:221:GLU:O	1:B:225:LYS:HG3	2.18	0.43
1:B:13:LYS:HE2	1:B:13:LYS:HB2	1.85	0.43
1:B:194:THR:O	1:B:198:VAL:HG23	2.19	0.42
2:D:14:G:O2'	2:D:15:G:H5'	2.19	0.42
1:B:78:TYR:HA	1:B:132:PHE:CE1	2.54	0.42
1:A:9:PRO:HA	3:A:2001:ANP:O2G	2.19	0.42
2:C:37:G:N2	2:C:38:A:C6	2.87	0.42
1:A:226:ILE:HG12	1:A:229:MSE:HE2	2.01	0.42
2:C:27:C:H2'	2:C:28:C:H6	1.85	0.42
2:D:47(N):G:O2'	2:D:48:C:H5'	2.20	0.42
1:A:39:ILE:HD13	1:A:57:SER:HB3	2.02	0.42
2:D:47(J):G:H2'	2:D:47(K):G:H8	1.84	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:32:C:C2	2:C:38:A:N6	2.87	0.41
1:A:2:LEU:O	1:A:97:TYR:HA	2.20	0.41
1:B:172:LYS:O	1:B:173:PHE:HB2	2.20	0.41
2:C:5(B):C:O2'	2:C:6:G:H5'	2.21	0.41
2:C:38:A:H2'	2:C:39:U:O5'	2.20	0.41
1:A:0:HIS:NE2	1:A:95:LYS:CE	2.83	0.41
1:A:228:LYS:NZ	5:A:1152:HOH:O	2.54	0.41
1:A:245:LEU:HD23	1:A:245:LEU:HA	1.90	0.41
1:B:194:THR:HG21	1:B:223:LEU:HD21	2.02	0.41
2:D:47(H):U:H5	5:D:1053:HOH:O	2.04	0.40
1:B:101:TYR:CZ	1:B:103:LYS:HG3	2.56	0.40
1:B:84:ARG:HB2	1:B:141:TRP:CH2	2.57	0.40
1:A:-2:HIS:HB3	1:A:-1:HIS:H	1.47	0.40
2:D:53:G:H2'	2:D:54:U:C6	2.56	0.40
1:A:158:GLU:HG3	1:A:162:LYS:HE3	2.02	0.40
1:B:117:GLY:O	1:B:118:GLU:C	2.60	0.40
2:D:47(B):C:H2'	2:D:47(C):C:C6	2.57	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	249/259 (96%)	239 (96%)	10 (4%)	0	100	100
1	B	235/259 (91%)	228 (97%)	6 (3%)	1 (0%)	38	54
All	All	484/518 (93%)	467 (96%)	16 (3%)	1 (0%)	51	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	186	ILE

### 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	238/241 (99%)	234 (98%)	4 (2%)	66	82
1	B	226/241 (94%)	223 (99%)	3 (1%)	73	87
All	All	464/482 (96%)	457 (98%)	7 (2%)	70	85

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

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	25	SER
1	A	75	ASP
1	A	187	SER
1	B	217	GLU
1	B	227	LYS
1	B	230	GLU

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	183	ASN
1	B	94	ASN
1	B	185	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	86/92 (93%)	12 (13%)	0
2	D	86/92 (93%)	11 (12%)	0
All	All	172/184 (93%)	23 (13%)	0

All (23) 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
2	C	38	A
2	C	39	U
2	C	47(F)	A
2	C	47(G)	G
2	C	47(I)	G
2	C	72	C
2	C	76	A
2	D	8	C
2	D	9	A
2	D	18	G
2	D	20	U
2	D	20(A)	C
2	D	33	U
2	D	47(F)	A
2	D	47(G)	G
2	D	47(H)	U
2	D	47(I)	G
2	D	74	C

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	29,33,33	1.58	5 (17%)	28,52,52	2.26	6 (21%)
3	ANP	B	2002	4	29,33,33	1.68	4 (13%)	28,52,52	1.96	5 (17%)

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	-	0/13/38/38	0/3/3/3
3	ANP	B	2002	4	-	0/13/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	ANP	PB-O2B	-2.88	1.48	1.56
3	B	2002	ANP	PG-O2G	2.26	1.62	1.56
3	A	2001	ANP	O4'-C4'	2.32	1.50	1.45
3	B	2002	ANP	PB-O1B	2.41	1.48	1.46
3	A	2001	ANP	PB-O1B	2.78	1.49	1.46
3	A	2001	ANP	PG-O1G	3.86	1.50	1.46
3	B	2002	ANP	O4'-C1'	4.16	1.47	1.41
3	A	2001	ANP	O4'-C1'	4.24	1.47	1.41
3	B	2002	ANP	PG-O1G	5.54	1.52	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	ANP	N3-C2-N1	-7.74	122.11	128.86
3	B	2002	ANP	N3-C2-N1	-7.27	122.53	128.86
3	A	2001	ANP	PA-O3A-PB	-3.37	120.49	132.38
3	A	2001	ANP	O1B-PB-N3B	-3.23	106.96	111.79
3	A	2001	ANP	O1G-PG-N3B	-3.19	107.01	111.79
3	A	2001	ANP	C4'-O4'-C1'	-3.11	106.46	109.77
3	B	2002	ANP	PA-O3A-PB	-2.60	123.20	132.38
3	B	2002	ANP	O1G-PG-N3B	-2.37	108.24	111.79
3	B	2002	ANP	O3G-PG-O1G	-2.12	108.01	113.41
3	B	2002	ANP	O2B-PB-O1B	3.97	118.11	109.87

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	ANP	O2B-PB-O1B	4.42	119.06	109.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	ANP	9	0
3	B	2002	ANP	3	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	247/259 (95%)	0.05	10 (4%) 39 38	28, 49, 99, 136	0
1	B	235/259 (90%)	0.18	20 (8%) 11 10	26, 51, 117, 135	0
2	C	88/92 (95%)	-0.33	5 (5%) 24 23	30, 64, 151, 199	0
2	D	88/92 (95%)	-0.06	6 (6%) 18 16	35, 78, 146, 178	0
All	All	658/702 (93%)	0.03	41 (6%) 21 20	26, 54, 122, 199	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	33	U	8.7
1	A	174	TYR	7.3
2	C	37	G	7.1
2	D	36	A	6.1
1	A	-2	HIS	5.9
1	A	176	LEU	5.6
1	B	186	ILE	5.5
2	D	47(G)	G	5.3
1	A	179	ASN	4.8
2	C	38	A	4.4
1	B	230	GLU	4.4
1	B	173	PHE	4.3
1	A	182	LYS	4.1
1	A	175	VAL	4.0
1	B	206	LYS	3.8
1	B	185	ASN	3.6
1	B	207	LEU	3.6
2	D	37	G	3.5
1	B	201	TYR	3.5
1	B	172	LYS	3.4
2	D	38	A	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	173	PHE	3.0
1	B	225	LYS	2.8
2	C	31	A	2.8
1	B	228	LYS	2.8
2	D	47(E)	G	2.7
1	B	232	VAL	2.7
1	B	227	LYS	2.7
1	A	236	ARG	2.6
1	B	208	ASP	2.6
2	C	76	A	2.4
1	B	243	ASP	2.3
1	B	242	LYS	2.3
1	B	231	GLU	2.3
1	A	183	ASN	2.2
1	B	215	VAL	2.2
1	B	119	LYS	2.2
1	B	248	TYR	2.2
2	C	32	C	2.2
1	A	178	GLU	2.1
1	B	192	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ANP	B	2002	31/31	0.94	0.17	0.78	37,59,74,79	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ANP	A	2001	31/31	0.93	0.25	0.62	46,92,102,102	0
4	MG	A	2003	1/1	0.93	0.05	-	59,59,59,59	0
4	MG	B	2004	1/1	0.95	0.10	-	41,41,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.