



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:21 AM GMT

PDB ID : 2SRC
Title : CRYSTAL STRUCTURE OF HUMAN TYROSINE-PROTEIN KINASE C-SRC, IN COMPLEX WITH AMP-PNP
Authors : Xu, W.; Doshi, A.; Lei, M.; Eck, M.J.; Harrison, S.C.
Deposited on : 1998-12-29
Resolution : 1.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

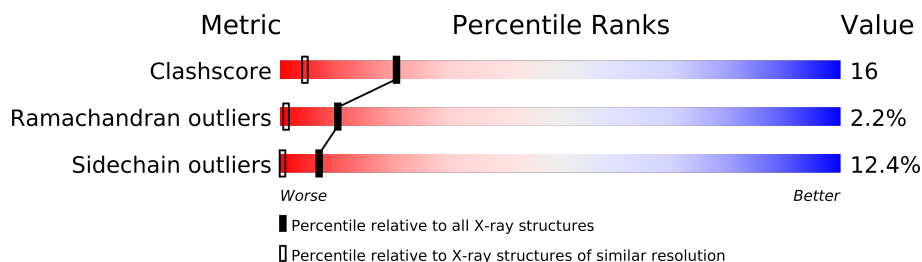
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 1.50 Å.


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	452	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3915 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.

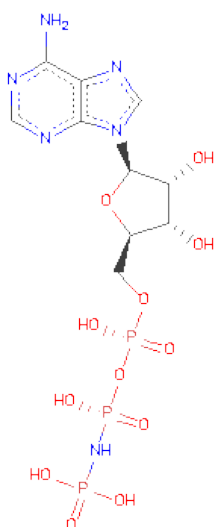
- Molecule 1 is a protein called TYROSINE-PROTEIN KINASE SRC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	450	3615	2296	614	685	1	19	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	527	PTR	TYR	MODIFIED RESIDUE	UNP P12931

- Molecule 2 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	269	Total 269	O 269	0	0

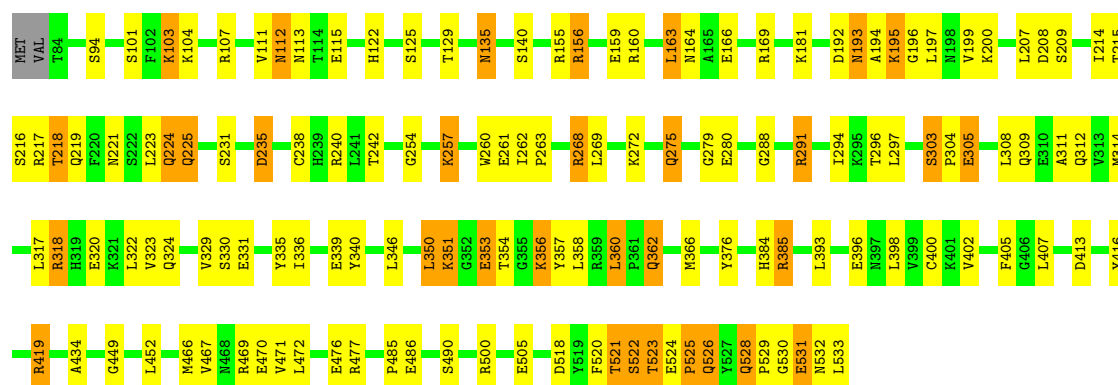
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: TYROSINE-PROTEIN KINASE SRC

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.59Å 72.97Å 172.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50	Depositor
% Data completeness (in resolution range)	89.1 (20.00-1.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.226 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3915	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.39	0/3683	0.60	0/4989

There are no bond length outliers.

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	3615	0	3543	111	0
2	A	31	0	13	1	0
3	A	269	0	0	14	0
All	All	3915	0	3556	112	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 16.

All (112) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:135:ASN:HD22	1:A:135:ASN:H	1.19	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:304:PRO:HB3	1:A:330:SER:O	1.76	0.84
1:A:261:GLU:HG2	3:A:1176:HOH:O	1.77	0.83
1:A:272:LYS:HZ1	1:A:275:GLN:HG3	1.42	0.83
1:A:524:GLU:N	1:A:525:PRO:HD3	1.99	0.77
1:A:260:TRP:HE1	1:A:312:GLN:HE22	1.32	0.77
1:A:525:PRO:HA	3:A:1166:HOH:O	1.84	0.77
1:A:192:ASP:HB3	1:A:195:LYS:HB3	1.66	0.76
1:A:115:GLU:HG2	1:A:257:LYS:NZ	2.01	0.76
1:A:135:ASN:HD22	1:A:135:ASN:N	1.86	0.72
1:A:115:GLU:HG2	1:A:257:LYS:HZ1	1.56	0.70
1:A:518:ASP:OD1	1:A:523:THR:HA	1.95	0.67
1:A:329:VAL:HB	1:A:335:TYR:HB2	1.76	0.66
1:A:272:LYS:HZ1	1:A:275:GLN:CG	2.09	0.65
1:A:466:MET:CE	1:A:471:VAL:HA	2.26	0.64
1:A:467:VAL:HG13	1:A:469:ARG:HG3	1.78	0.64
1:A:268:ARG:NH1	1:A:288:GLY:H	1.96	0.64
1:A:466:MET:HE1	1:A:471:VAL:HA	1.80	0.64
1:A:366:MET:HG2	1:A:400:CYS:SG	2.38	0.64
1:A:384:HIS:O	1:A:385:ARG:HB2	1.99	0.62
1:A:485:PRO:O	1:A:486:GLU:HB2	1.98	0.62
1:A:135:ASN:H	1:A:135:ASN:ND2	1.93	0.62
1:A:268:ARG:HH12	1:A:288:GLY:H	1.48	0.61
1:A:268:ARG:HH11	1:A:268:ARG:CG	2.14	0.60
1:A:297:LEU:HD21	1:A:336:ILE:HD12	1.84	0.60
1:A:214:ILE:HA	3:A:1211:HOH:O	2.02	0.59
1:A:279:GLY:HA3	1:A:296:THR:O	2.03	0.57
1:A:500:ARG:HD3	1:A:505:GLU:HB3	1.87	0.56
1:A:192:ASP:CB	1:A:195:LYS:HB3	2.34	0.56
1:A:309:GLN:HB3	3:A:1089:HOH:O	2.06	0.56
1:A:303:SER:OG	1:A:305:GLU:HG2	2.07	0.55
1:A:323:VAL:HG21	1:A:393:LEU:HD12	1.88	0.55
1:A:297:LEU:HD21	1:A:336:ILE:CD1	2.36	0.55
1:A:360:LEU:HD13	1:A:520:PHE:HZ	1.70	0.55
1:A:155:ARG:HD2	1:A:524:GLU:HG3	1.88	0.55
1:A:311:ALA:HA	1:A:314:MET:CE	2.37	0.54
1:A:156:ARG:HD2	3:A:1067:HOH:O	2.07	0.54
1:A:358:LEU:HD23	1:A:362:GLN:HE21	1.73	0.53
1:A:518:ASP:CG	1:A:523:THR:HA	2.29	0.53
1:A:524:GLU:HG2	3:A:1088:HOH:O	2.07	0.53
1:A:346:LEU:HG	1:A:350:LEU:HD22	1.91	0.53
1:A:467:VAL:HG12	1:A:470:GLU:OE2	2.10	0.52
1:A:419:ARG:HG2	1:A:434:ALA:HA	1.91	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:224:GLN:H	1:A:224:GLN:NE2	2.08	0.51
1:A:524:GLU:N	1:A:525:PRO:CD	2.70	0.51
1:A:523:THR:C	1:A:525:PRO:HD3	2.30	0.51
1:A:467:VAL:HG12	1:A:470:GLU:HG2	1.91	0.51
1:A:200:LYS:HG3	1:A:238:CYS:SG	2.50	0.51
1:A:268:ARG:HG2	1:A:268:ARG:NH1	2.25	0.51
1:A:192:ASP:O	1:A:196:GLY:N	2.42	0.50
1:A:231:SER:O	1:A:240:ARG:HD2	2.11	0.50
1:A:214:ILE:HG12	3:A:1211:HOH:O	2.10	0.50
1:A:269:LEU:HD23	1:A:294:ILE:HD13	1.92	0.50
1:A:268:ARG:NH1	1:A:268:ARG:CG	2.74	0.49
1:A:164:ASN:HD21	1:A:166:GLU:HG3	1.77	0.49
1:A:103:LYS:HG3	1:A:104:LYS:N	2.27	0.49
1:A:353:GLU:HG3	1:A:354:THR:N	2.29	0.48
1:A:522:SER:C	1:A:524:GLU:H	2.17	0.47
1:A:314:MET:HA	1:A:317:LEU:HD12	1.97	0.47
1:A:291:ARG:HD2	3:A:1238:HOH:O	2.14	0.47
1:A:466:MET:HE2	1:A:471:VAL:HA	1.95	0.47
1:A:311:ALA:HA	1:A:314:MET:HE1	1.97	0.47
1:A:215:THR:HG22	3:A:1049:HOH:O	2.13	0.47
1:A:269:LEU:CD2	1:A:294:ILE:HD13	2.45	0.46
1:A:477:ARG:HB3	1:A:477:ARG:NH1	2.30	0.46
1:A:322:LEU:CD2	1:A:402:VAL:HB	2.45	0.46
1:A:318:ARG:NH2	1:A:376:TYR:OH	2.47	0.46
1:A:254:GLY:H	1:A:324:GLN:HE22	1.63	0.46
1:A:314:MET:HB2	1:A:314:MET:HE2	1.54	0.46
1:A:413:ASP:HB3	1:A:416:TYR:HB3	1.96	0.46
1:A:528:GLN:HA	1:A:528:GLN:NE2	2.30	0.46
1:A:305:GLU:H	1:A:305:GLU:CD	2.19	0.45
1:A:322:LEU:HD23	1:A:402:VAL:HB	1.98	0.45
1:A:531:GLU:O	1:A:531:GLU:HG2	2.16	0.45
1:A:163:LEU:CD1	1:A:199:VAL:HG23	2.46	0.45
1:A:336:ILE:HD13	1:A:407:LEU:HD11	1.98	0.45
1:A:122:HIS:CD2	1:A:129:THR:HG22	2.52	0.45
1:A:164:ASN:ND2	1:A:166:GLU:HG3	2.31	0.44
1:A:163:LEU:HD13	1:A:199:VAL:HG23	1.99	0.44
1:A:193:ASN:HD22	1:A:194:ALA:N	2.15	0.44
1:A:272:LYS:HE2	1:A:280:GLU:OE2	2.17	0.44
1:A:356:LYS:HG3	1:A:357:TYR:N	2.32	0.44
1:A:193:ASN:HD22	1:A:193:ASN:N	2.14	0.43
1:A:221:ASN:HB2	1:A:225:GLN:HE22	1.83	0.43
1:A:94:SER:N	1:A:101:SER:OG	2.46	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:268:ARG:NH1	1:A:288:GLY:N	2.64	0.43
1:A:384:HIS:CD2	1:A:405:PHE:HB3	2.53	0.43
1:A:520:PHE:O	1:A:521:THR:C	2.57	0.43
1:A:217:ARG:NH1	1:A:235:ASP:OD2	2.48	0.43
1:A:155:ARG:HD3	3:A:1268:HOH:O	2.18	0.43
1:A:311:ALA:HA	1:A:314:MET:HE2	1.99	0.43
1:A:159:GLU:O	1:A:163:LEU:HD22	2.18	0.43
1:A:351:LYS:HE3	3:A:1245:HOH:O	2.17	0.43
1:A:113:ASN:C	1:A:115:GLU:H	2.22	0.43
1:A:240:ARG:O	1:A:242:THR:HG23	2.19	0.43
1:A:275:GLN:HG2	1:A:280:GLU:HG2	2.00	0.42
1:A:135:ASN:ND2	1:A:135:ASN:N	2.58	0.42
1:A:224:GLN:HE21	1:A:224:GLN:H	1.67	0.42
1:A:217:ARG:HD2	1:A:218:THR:OG1	2.18	0.42
1:A:197:LEU:HD21	3:A:1150:HOH:O	2.20	0.42
1:A:351:LYS:HG2	1:A:351:LYS:H	1.55	0.42
1:A:323:VAL:HG13	1:A:339:GLU:HG2	2.00	0.42
1:A:94:SER:H	1:A:101:SER:HG	1.63	0.42
1:A:291:ARG:NH1	3:A:1238:HOH:O	2.52	0.41
1:A:449:GLY:O	1:A:452:LEU:HB2	2.20	0.41
2:A:1:ANP:H3'	3:A:1230:HOH:O	2.19	0.41
1:A:111:VAL:O	1:A:112:ASN:HB2	2.20	0.41
1:A:193:ASN:C	1:A:193:ASN:ND2	2.74	0.41
1:A:262:ILE:HB	1:A:263:PRO:HD2	2.03	0.41
1:A:467:VAL:CG1	1:A:470:GLU:HG2	2.51	0.40
1:A:291:ARG:HD3	1:A:340:TYR:CD2	2.56	0.40
1:A:268:ARG:HG2	1:A:268:ARG:HH11	1.82	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	447/452 (99%)	418 (94%)	19 (4%)	10 (2%)	10 1

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	LYS
1	A	521	THR
1	A	112	ASN
1	A	207	LEU
1	A	522	SER
1	A	525	PRO
1	A	526	GLN
1	A	523	THR
1	A	529	PRO
1	A	530	GLY

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	388/391 (99%)	340 (88%)	48 (12%)	7 0

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LYS
1	A	107	ARG
1	A	125	SER
1	A	135	ASN
1	A	140	SER
1	A	156	ARG
1	A	160	ARG
1	A	163	LEU
1	A	169	ARG
1	A	181	LYS
1	A	193	ASN
1	A	208	ASP
1	A	209	SER
1	A	216	SER
1	A	218	THR
1	A	219	GLN
1	A	223	LEU

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Mol	Chain	Res	Type
1	A	224	GLN
1	A	225	GLN
1	A	235	ASP
1	A	257	LYS
1	A	268	ARG
1	A	275	GLN
1	A	291	ARG
1	A	303	SER
1	A	305	GLU
1	A	308	LEU
1	A	318	ARG
1	A	320	GLU
1	A	331	GLU
1	A	350	LEU
1	A	351	LYS
1	A	353	GLU
1	A	356	LYS
1	A	360	LEU
1	A	362	GLN
1	A	385	ARG
1	A	396	GLU
1	A	398	LEU
1	A	419	ARG
1	A	472	LEU
1	A	476	GLU
1	A	490	SER
1	A	526	GLN
1	A	528	GLN
1	A	531	GLU
1	A	532	ASN
1	A	533	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	135	ASN
1	A	164	ASN
1	A	193	ASN
1	A	219	GLN
1	A	224	GLN
1	A	225	GLN

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Mol	Chain	Res	Type
1	A	312	GLN
1	A	324	GLN
1	A	362	GLN
1	A	526	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	PTR	A	527	1	16,16,17	5.46	4 (25%)	20,22,24	2.88	2 (10%)

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
1	PTR	A	527	1	-	0/9/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	PTR	O-C	16.91	1.23	1.11
1	A	527	PTR	P-OH	11.75	1.78	1.60
1	A	527	PTR	OH-CZ	6.52	1.57	1.40
1	A	527	PTR	CA-C	2.22	1.52	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	PTR	C-CA-N	-10.83	103.01	113.83
1	A	527	PTR	P-OH-CZ	6.02	140.54	123.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	ANP	A	1	-	33,33,33	2.45	7 (21%)	51,52,52	3.03	19 (37%)

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	ANP	A	1	-	-	1/18/38/38	0/1/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	ANP	PG-N3B	7.30	1.70	1.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	ANP	PB-O3A	6.77	1.68	1.59
2	A	1	ANP	PG-O1G	5.10	1.52	1.46
2	A	1	ANP	PB-O1B	3.74	1.50	1.46
2	A	1	ANP	C2'-C1'	-3.65	1.48	1.53
2	A	1	ANP	PB-N3B	-3.36	1.61	1.64
2	A	1	ANP	PB-O2B	-2.83	1.46	1.55

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ANP	O4'-C1'-N9	10.44	118.15	108.44
2	A	1	ANP	C4'-O4'-C1'	8.58	119.07	109.75
2	A	1	ANP	N3-C4-N9	6.89	137.88	125.43
2	A	1	ANP	O1B-PB-N3B	-6.18	102.48	111.83
2	A	1	ANP	O1G-PG-N3B	-5.25	103.90	111.83
2	A	1	ANP	O4'-C1'-C2'	-4.35	100.10	106.77
2	A	1	ANP	N3-C2-N1	-4.34	125.08	128.71
2	A	1	ANP	C5-C4-N3	-4.22	116.52	125.70
2	A	1	ANP	O3A-PB-N3B	4.16	118.14	106.59
2	A	1	ANP	O2B-PB-N3B	4.12	117.79	106.61
2	A	1	ANP	PA-O3A-PB	3.43	143.52	131.81
2	A	1	ANP	C3'-C2'-C1'	3.18	105.89	100.91
2	A	1	ANP	O4'-C4'-C3'	-2.72	99.65	105.17
2	A	1	ANP	C2-N3-C4	2.55	121.28	114.01
2	A	1	ANP	C6-C5-C4	2.53	121.89	117.25
2	A	1	ANP	O3'-C3'-C4'	-2.18	104.64	111.08
2	A	1	ANP	O2'-C2'-C1'	-2.09	104.89	111.23
2	A	1	ANP	O3'-C3'-C2'	-2.03	105.22	111.83
2	A	1	ANP	O3G-PG-O2G	2.03	113.49	107.66

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	ANP	O1B-PB-N3B-PG

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.