



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2017 – 06:07 AM EDT

PDB ID : 3DGR
Title : Crystal structure of human NAMPT complexed with ADP analogue
Authors : Ho, M.; Burgos, E.S.; Almo, S.C.; Schramm, V.L.
Deposited on : unknown
Resolution : 2.10 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

<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 : rb-20030345
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) : rb-20030345

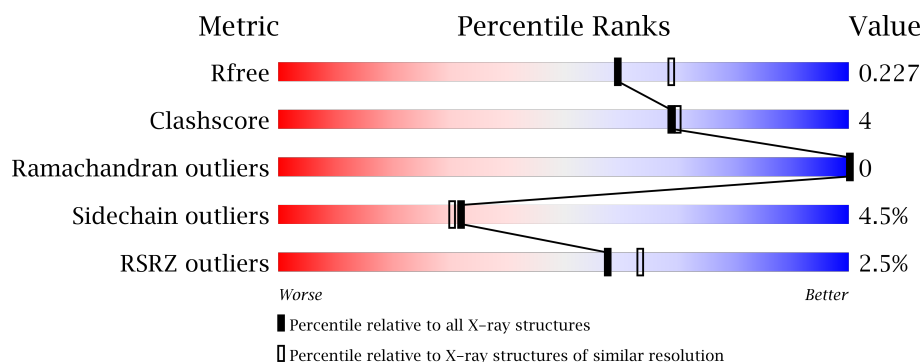
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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. 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	484	<div> <div>3%</div> <div>86%</div> <div>8%</div> <div>• •</div> </div>
1	B	484	<div> <div>2%</div> <div>85%</div> <div>10%</div> <div>• •</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
2	A12	A	501	-	-	-	X
2	A12	B	501	-	-	-	X

2 Entry composition [i](#)

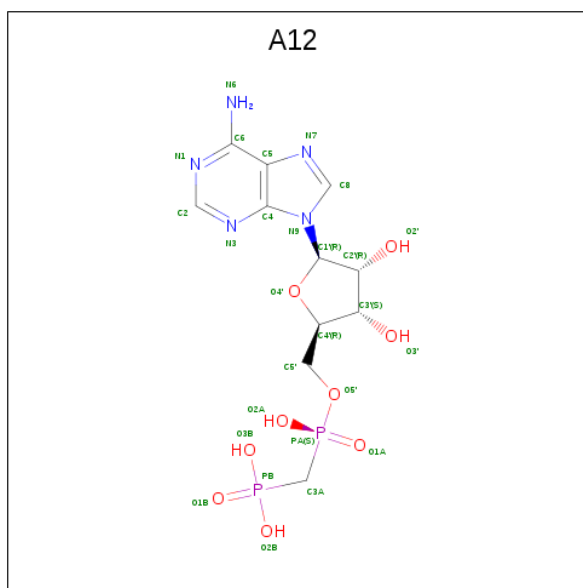
There are 3 unique types of molecules in this entry. The entry contains 7786 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3711	2388	613	703	7			
1	B	464	Total	C	N	O	S	0	1	0
			3717	2393	614	703	7			

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: A12) (formula: $C_{11}H_{17}N_5O_9P_2$).

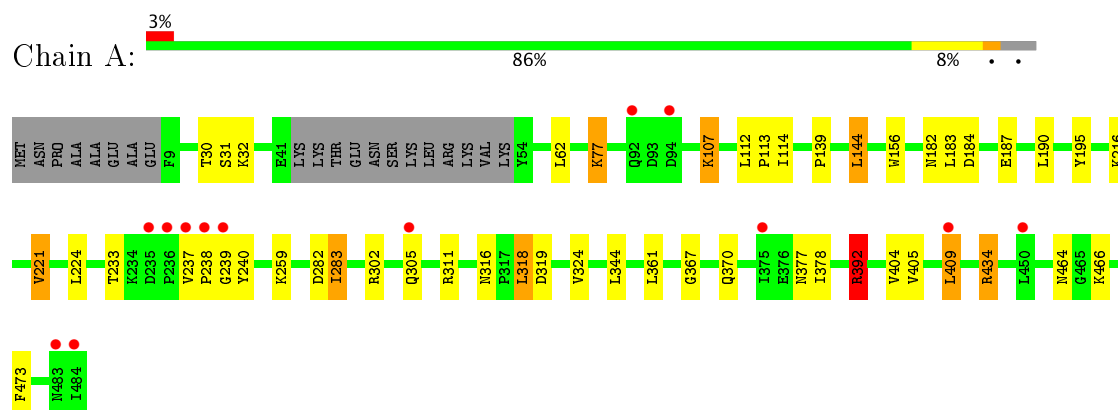


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	151	Total 151	O 151	0	0
3	B	153	Total 153	O 153	0	0

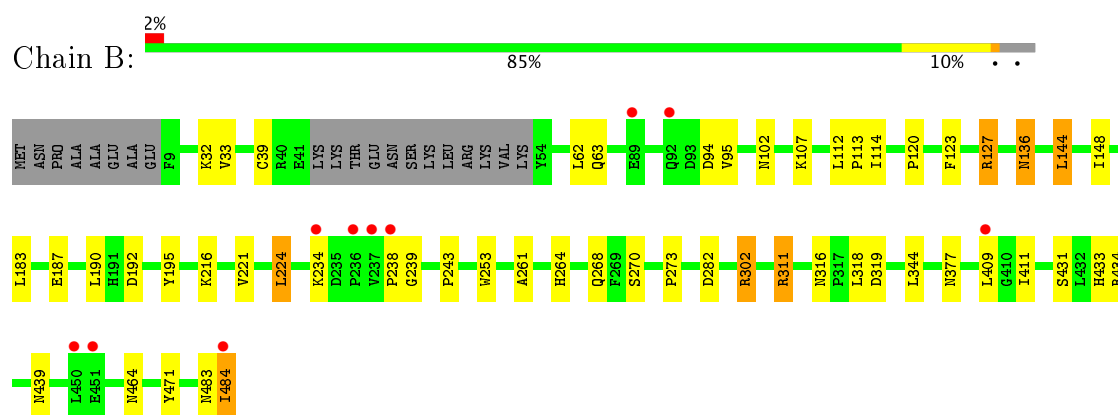
3 Residue-property plots [i](#)

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

- Molecule 1: Nicotinamide phosphoribosyltransferase



- Molecule 1: Nicotinamide phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.29 Å 107.23 Å 82.66 Å 90.00° 96.41° 90.00°	Depositor
Resolution (Å)	19.92 – 2.10 19.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (19.92-2.10) 94.1 (19.92-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.09 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.225 0.182 , 0.227	Depositor DCC
R_{free} test set	2970 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7786	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A12

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	0.73	0/3799	0.75	6/5149 (0.1%)
1	B	0.76	0/3808	0.73	5/5160 (0.1%)
All	All	0.75	0/7607	0.74	11/10309 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	B	127	ARG	NE-CZ-NH1	-7.81	116.40	120.30
1	A	409	LEU	CA-CB-CG	7.22	131.90	115.30
1	A	392	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	B	311	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	A	282	ASP	CB-CG-OD1	6.29	123.96	118.30
1	B	282	ASP	CB-CG-OD1	5.86	123.58	118.30
1	A	302	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	B	302	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	192	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	311	ARG	NE-CZ-NH2	-5.15	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3711	0	3686	30	0
1	B	3717	0	3699	34	0
2	A	27	0	14	0	0
2	B	27	0	14	0	0
3	A	151	0	0	0	0
3	B	153	0	0	2	0
All	All	7786	0	7413	64	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 (64) 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:A:221:VAL:HA	1:A:224:LEU:HD23	1.53	0.90
1:A:182:ASN:HD22	1:A:184:ASP:H	1.25	0.84
1:B:344:LEU:H	1:B:377:ASN:HD21	1.25	0.80
1:A:316:ASN:HD22	1:A:319:ASP:H	1.33	0.76
1:B:316:ASN:HD22	1:B:319:ASP:H	1.33	0.75
1:A:344:LEU:H	1:A:377:ASN:HD21	1.35	0.72
1:A:107:LYS:HE2	1:A:107:LYS:HA	1.72	0.71
1:A:77:LYS:O	1:A:77:LYS:HD2	1.92	0.70
1:A:224:LEU:HD12	1:A:238:PRO:HD2	1.74	0.69
1:B:224:LEU:HD12	1:B:238:PRO:HD2	1.74	0.69
1:B:63:GLN:HE22	1:B:471:TYR:H	1.42	0.68
1:B:344:LEU:H	1:B:377:ASN:ND2	1.94	0.65
1:B:483:ASN:O	1:B:484:ILE:HG12	1.96	0.65
1:B:114:ILE:CD1	1:B:144:LEU:HD13	2.26	0.64
1:B:114:ILE:HD13	1:B:148:ILE:HD13	1.80	0.63
1:B:311:ARG:NH2	3:B:548:HOH:O	2.26	0.63
1:B:136:ASN:H	1:B:136:ASN:HD22	1.46	0.62
1:A:113:PRO:HA	1:A:464:ASN:HD22	1.64	0.61
1:B:113:PRO:HA	1:B:464:ASN:HD22	1.68	0.58
1:A:216:LYS:O	1:A:239:GLY:HA2	2.04	0.57
1:B:224:LEU:HD11	1:B:239:GLY:HA3	1.85	0.57
1:B:224:LEU:H	1:B:224:LEU:HD22	1.70	0.56
1:A:344:LEU:H	1:A:377:ASN:ND2	2.04	0.55
1:A:31:SER:HB2	1:A:139:PRO:HB3	1.87	0.55
1:A:107:LYS:HE2	1:A:107:LYS:CA	2.37	0.55
1:A:237:VAL:HG23	1:A:240:TYR:CE2	2.44	0.53
1:A:32:LYS:O	1:A:404:VAL:HG23	2.08	0.53
1:B:270:SER:HA	1:B:302:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ASN:C	1:B:484:ILE:HG12	2.30	0.52
1:B:224:LEU:H	1:B:224:LEU:CD2	2.24	0.51
1:B:114:ILE:HD13	1:B:148:ILE:CD1	2.40	0.51
1:A:182:ASN:ND2	1:A:184:ASP:H	2.03	0.50
1:B:33:VAL:H	1:B:136:ASN:HD21	1.59	0.50
1:B:216:LYS:O	1:B:239:GLY:HA2	2.11	0.50
1:B:136:ASN:ND2	1:B:136:ASN:H	2.08	0.50
1:A:114:ILE:HG12	1:A:144:LEU:HD13	1.94	0.49
1:B:32:LYS:HA	1:B:136:ASN:HD21	1.77	0.49
1:B:114:ILE:HD11	1:B:144:LEU:HD13	1.95	0.49
1:A:112:LEU:O	1:A:464:ASN:HA	2.13	0.49
1:A:283:ILE:CD1	1:A:324:VAL:CG2	2.91	0.48
1:B:224:LEU:N	1:B:224:LEU:HD22	2.29	0.48
1:A:113:PRO:HD2	1:A:144:LEU:CD1	2.44	0.47
1:B:33:VAL:H	1:B:136:ASN:ND2	2.13	0.47
1:A:30:THR:HG23	1:A:404:VAL:CG2	2.44	0.47
1:B:439:ASN:HB3	3:B:651:HOH:O	2.14	0.47
1:B:243:PRO:HD2	1:B:273:PRO:O	2.15	0.46
1:A:224:LEU:HD12	1:A:238:PRO:CD	2.45	0.46
1:B:431:SER:OG	1:B:433:HIS:HE1	1.99	0.46
1:A:32:LYS:HB3	1:A:405:VAL:HB	1.98	0.45
1:A:113:PRO:HA	1:A:464:ASN:ND2	2.29	0.45
1:B:264:HIS:O	1:B:268:GLN:HG2	2.16	0.45
1:A:156:TRP:CG	1:A:392:ARG:HG3	2.52	0.44
1:A:316:ASN:ND2	1:A:319:ASP:H	2.09	0.44
1:B:187:GLU:HG3	1:B:216:LYS:HD2	1.99	0.44
1:A:434:ARG:HD3	1:A:434:ARG:HA	1.73	0.43
1:A:283:ILE:HD11	1:A:324:VAL:CG2	2.48	0.42
1:B:120:PRO:O	1:B:123:PHE:HB2	2.18	0.42
1:B:39:CYS:O	1:B:127:ARG:HG2	2.19	0.42
1:A:318:LEU:HD21	1:A:367:GLY:HA3	2.02	0.42
1:B:253:TRP:CG	1:B:261:ALA:HB2	2.55	0.42
1:A:233:THR:CG2	1:A:473:PHE:HB3	2.50	0.41
1:B:112:LEU:O	1:B:464:ASN:HA	2.21	0.40
1:B:221:VAL:HG23	1:B:221:VAL:H	1.49	0.40
1:A:113:PRO:HD2	1:A:144:LEU:HD12	2.04	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	460/484 (95%)	446 (97%)	14 (3%)	0	100	100
1	B	461/484 (95%)	444 (96%)	17 (4%)	0	100	100
All	All	921/968 (95%)	890 (97%)	31 (3%)	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	408/425 (96%)	388 (95%)	20 (5%)	29	26
1	B	409/425 (96%)	392 (96%)	17 (4%)	34	33
All	All	817/850 (96%)	780 (96%)	37 (4%)	32	30

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	77	LYS
1	A	107	LYS
1	A	144	LEU
1	A	183	LEU
1	A	187	GLU
1	A	190	LEU
1	A	195	TYR

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Mol	Chain	Res	Type
1	A	221	VAL
1	A	259	LYS
1	A	283	ILE
1	A	305	GLN
1	A	318	LEU
1	A	361	LEU
1	A	370	GLN
1	A	378	ILE
1	A	392	ARG
1	A	409	LEU
1	A	434	ARG
1	A	466	LYS
1	B	62	LEU
1	B	94	ASP
1	B	95	VAL
1	B	102	ASN
1	B	107	LYS
1	B	136	ASN
1	B	144	LEU
1	B	183	LEU
1	B	190	LEU
1	B	195	TYR
1	B	224	LEU
1	B	234	LYS
1	B	318	LEU
1	B	409	LEU
1	B	411	ILE
1	B	434	ARG
1	B	484	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	182	ASN
1	A	316	ASN
1	A	362	GLN
1	A	377	ASN
1	A	464	ASN
1	B	63	GLN
1	B	97	ASN
1	B	129	ASN

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Mol	Chain	Res	Type
1	B	136	ASN
1	B	168	GLN
1	B	316	ASN
1	B	370	GLN
1	B	377	ASN
1	B	396	ASN
1	B	433	HIS
1	B	464	ASN
1	B	479	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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](#)

2 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	A12	A	501	-	24,29,29	2.97	5 (20%)	26,45,45	2.04	4 (15%)
2	A12	B	501	-	24,29,29	2.79	4 (16%)	26,45,45	2.03	3 (11%)

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	A12	A	501	-	-	0/12/32/32	0/3/3/3
2	A12	B	501	-	-	0/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A12	PB-O3B	-2.62	1.48	1.54
2	B	501	A12	PA-O5'	2.35	1.60	1.57
2	A	501	A12	PA-O1A	2.84	1.58	1.51
2	B	501	A12	PA-O1A	3.19	1.59	1.51
2	A	501	A12	PA-O5'	3.35	1.61	1.57
2	B	501	A12	PA-O2A	8.68	1.77	1.56
2	B	501	A12	PB-O2B	9.14	1.76	1.54
2	A	501	A12	PB-O2B	9.22	1.76	1.54
2	A	501	A12	PA-O2A	9.33	1.78	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	A12	N3-C2-N1	-8.49	121.46	128.86
2	A	501	A12	N3-C2-N1	-8.26	121.67	128.86
2	A	501	A12	C4-C5-N7	-2.70	106.80	109.41
2	B	501	A12	O2B-PB-O1B	-2.45	105.75	112.32
2	B	501	A12	C4-C5-N7	-2.08	107.40	109.41
2	A	501	A12	O2B-PB-O1B	-2.04	106.86	112.32
2	A	501	A12	O2B-PB-C3A	2.42	112.26	106.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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	464/484 (95%)	-0.13	13 (2%) 53 60	19, 31, 46, 65	0
1	B	464/484 (95%)	-0.13	10 (2%) 62 67	21, 31, 46, 65	0
All	All	928/968 (95%)	-0.13	23 (2%) 58 63	19, 31, 46, 65	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	236	PRO	4.8
1	A	236	PRO	4.6
1	A	484	ILE	4.3
1	B	238	PRO	4.2
1	A	239	GLY	3.9
1	B	484	ILE	3.4
1	A	238	PRO	3.4
1	A	92	GLN	3.1
1	B	92	GLN	2.9
1	A	94	ASP	2.8
1	B	409	LEU	2.7
1	B	237	VAL	2.7
1	A	305	GLN	2.6
1	A	237	VAL	2.5
1	B	450	LEU	2.4
1	A	483	ASN	2.3
1	B	451	GLU	2.3
1	A	235	ASP	2.2
1	A	375	ILE	2.1
1	B	89	GLU	2.1
1	A	450	LEU	2.0
1	A	409	LEU	2.0
1	B	234	LYS	2.0

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, 95th 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(\AA^2)	Q<0.9
2	A12	A	501	27/27	0.95	0.16	2.92	38,43,47,49	0
2	A12	B	501	27/27	0.94	0.14	2.43	35,40,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.