



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:58 AM GMT

PDB ID : 2JHR
Title : CRYSTAL STRUCTURE OF MYOSIN-2 MOTOR DOMAIN IN COMPLEX WITH ADP-METAVANADATE AND PENTABROMOPSEUDILIN
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Deposited on : 2008-03-25
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

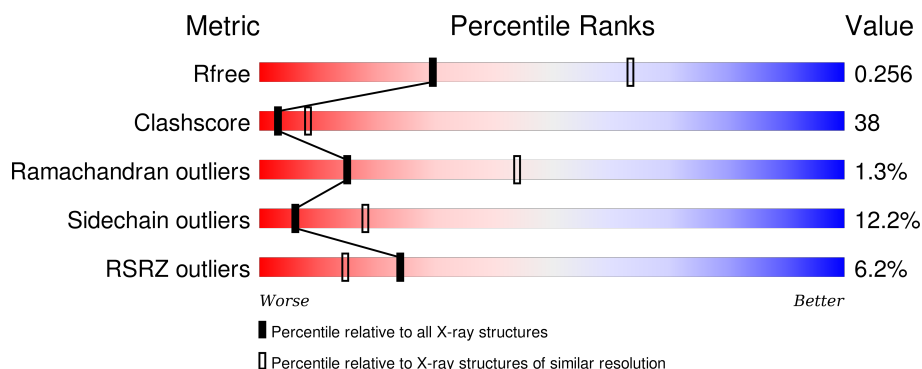
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	788	

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
4	PBQ	A	1780	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6761 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 MYOSIN-2 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	776	Total	C	N	O	S	0	0	0
			6239	3961	1076	1185	17			

There are 28 discrepancies between the modelled and reference sequences:

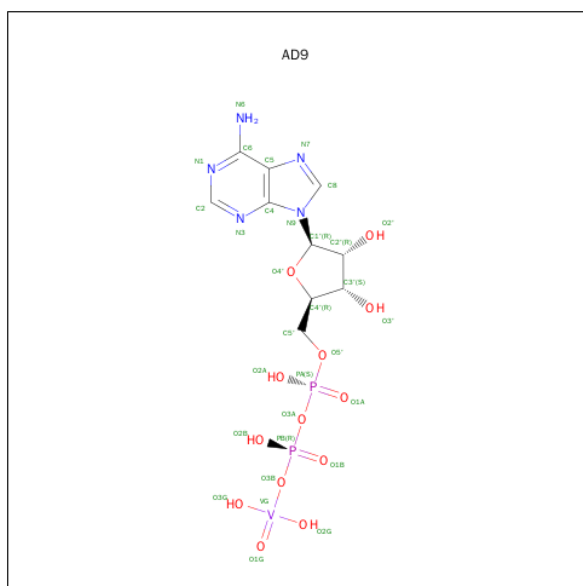
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP P08799
A	-9	HIS	-	EXPRESSION TAG	UNP P08799
A	-8	HIS	-	EXPRESSION TAG	UNP P08799
A	-7	HIS	-	EXPRESSION TAG	UNP P08799
A	-6	HIS	-	EXPRESSION TAG	UNP P08799
A	-5	HIS	-	EXPRESSION TAG	UNP P08799
A	-4	HIS	-	EXPRESSION TAG	UNP P08799
A	-3	HIS	-	EXPRESSION TAG	UNP P08799
A	-2	ASP	-	EXPRESSION TAG	UNP P08799
A	-1	GLY	-	EXPRESSION TAG	UNP P08799
A	0	THR	-	EXPRESSION TAG	UNP P08799
A	1	GLU	-	EXPRESSION TAG	UNP P08799
A	762	LEU	-	EXPRESSION TAG	UNP P08799
A	763	GLU	-	EXPRESSION TAG	UNP P08799
A	764	SER	-	EXPRESSION TAG	UNP P08799
A	765	ASN	-	EXPRESSION TAG	UNP P08799
A	766	GLU	-	EXPRESSION TAG	UNP P08799
A	767	PRO	-	EXPRESSION TAG	UNP P08799
A	768	PRO	-	EXPRESSION TAG	UNP P08799
A	769	MET	-	EXPRESSION TAG	UNP P08799
A	770	ASP	-	EXPRESSION TAG	UNP P08799
A	771	PHE	-	EXPRESSION TAG	UNP P08799
A	772	ASP	-	EXPRESSION TAG	UNP P08799
A	773	ASP	-	EXPRESSION TAG	UNP P08799
A	774	ASP	-	EXPRESSION TAG	UNP P08799
A	775	ILE	-	EXPRESSION TAG	UNP P08799
A	776	PRO	-	EXPRESSION TAG	UNP P08799

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Chain	Residue	Modelled	Actual	Comment	Reference
A	777	PHE	-	EXPRESSION TAG	UNP P08799

- Molecule 2 is ADP METAVANADATE (three-letter code: AD9) (formula: $C_{10}H_{16}N_5O_{13}P_2V$).

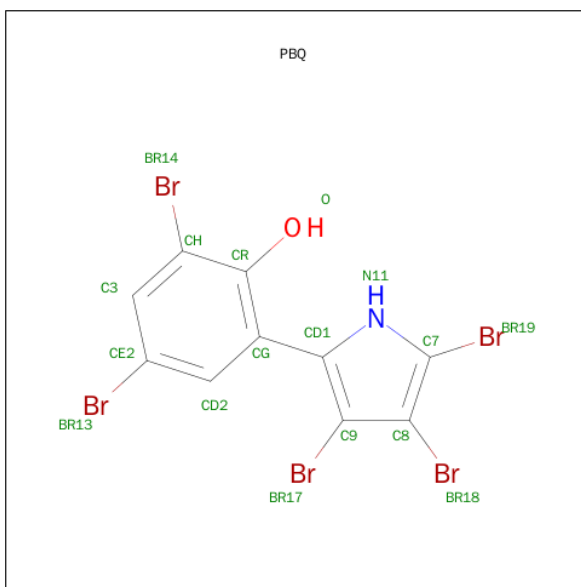


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	V	0	0
			31	10	5	13	2	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PENTABROMOPSEUDILIN (three-letter code: PBQ) (formula: $C_{10}H_4Br_5NO$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	Br	C	N	O	0	0
			17	5	10	1	1		

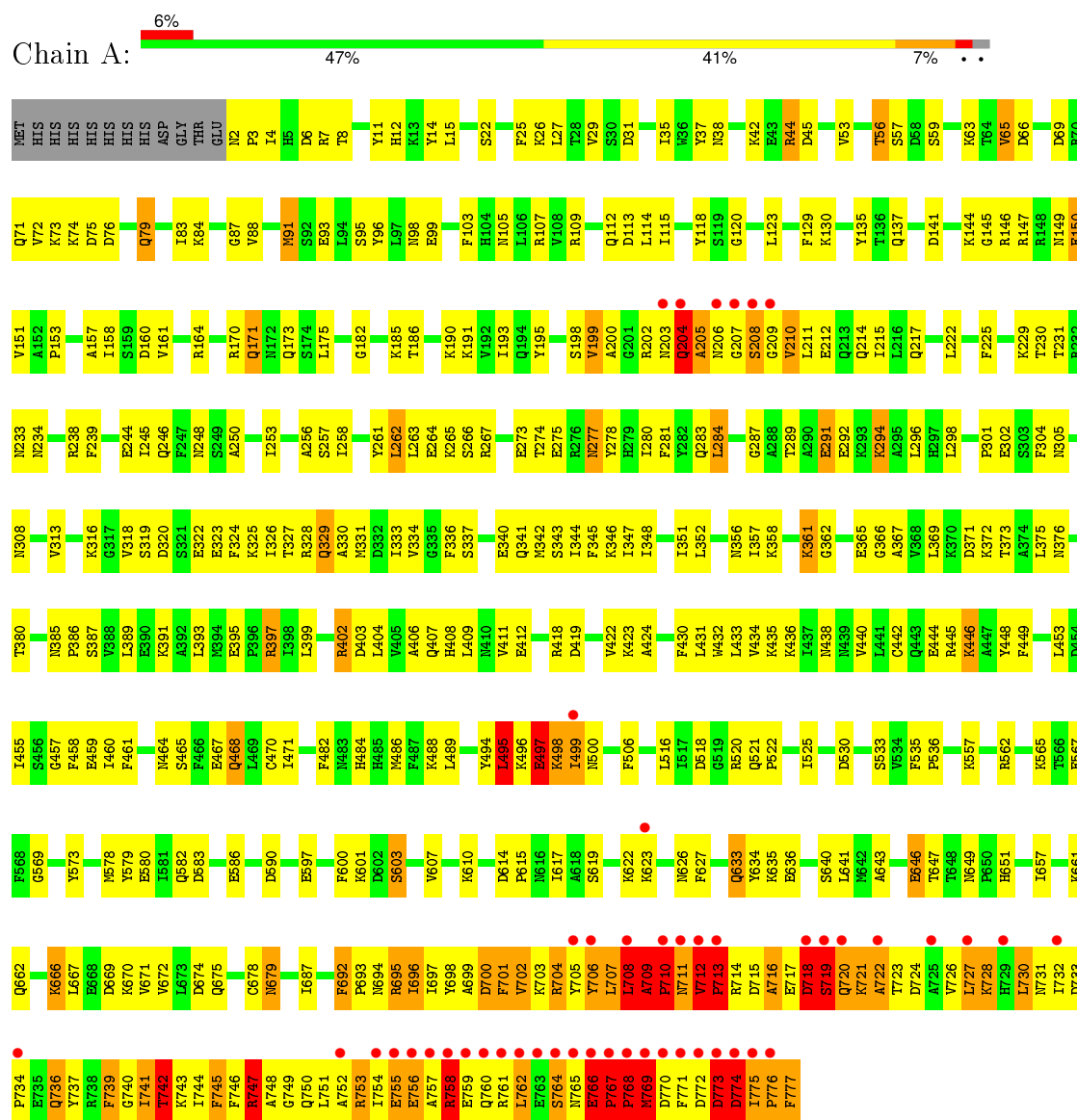
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	473	Total O 473 473	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.

• Molecule 1: MYOSIN-2 HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	89.76Å 150.46Å 154.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 77.08 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 76.5 (77.08-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.265 0.222 , 0.256	Depositor DCC
R_{free} test set	1232 reflections (6.42%)	DCC
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 155.4	EDS
Estimated twinning fraction	0.011 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.027 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 198675 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6761	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, PBQ, AD9

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	0.57	5/6364 (0.1%)	0.97	44/8590 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	713	PRO	N-CD	19.30	1.74	1.47
1	A	747	ARG	C-N	-7.76	1.16	1.34
1	A	710	PRO	N-CD	7.02	1.57	1.47
1	A	767	PRO	N-CD	6.39	1.56	1.47
1	A	718	ASP	C-N	-5.10	1.22	1.34

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASN	CB-CA-C	-15.77	78.87	110.40
1	A	739	PHE	CB-CA-C	-15.21	79.97	110.40
1	A	708	LEU	CB-CA-C	14.16	137.10	110.20
1	A	757	ALA	CB-CA-C	13.91	130.97	110.10
1	A	722	ALA	CB-CA-C	-13.73	89.50	110.10

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	711	ASN	Peptide
1	A	712	VAL	Peptide
1	A	718	ASP	Mainchain
1	A	747	ARG	Mainchain
1	A	767	PRO	Peptide

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	6239	0	6175	471	0
2	A	31	0	14	2	0
3	A	1	0	0	0	0
4	A	17	0	3	11	0
5	A	473	0	0	35	0
All	All	6761	0	6192	474	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 38.

The worst 5 of 474 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:713:PRO:CD	1:A:713:PRO:N	1.74	1.44
1:A:431:LEU:HD13	4:A:1780:PBQ:BR18	1.95	1.20
1:A:773:ASP:H	1:A:775:ILE:HG22	1.10	1.16
1:A:496:LYS:O	1:A:498:LYS:HG2	1.47	1.12
1:A:739:PHE:HA	1:A:744:ILE:HG13	1.31	1.12

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	774/788 (98%)	692 (89%)	72 (9%)	10 (1%)	15	44

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	GLU
1	A	713	PRO
1	A	709	ALA
1	A	710	PRO
1	A	766	GLU

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	680/691 (98%)	597 (88%)	83 (12%)	6	18

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	446	LYS
1	A	646	GLU
1	A	766	GLU
1	A	468	GLN
1	A	499	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	408	HIS

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Mol	Chain	Res	Type
1	A	679	ASN
1	A	407	GLN
1	A	443	GLN

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](#)

Of 3 ligands modelled in this entry, 1 is 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	$\# Z > 2$
2	AD9	A	1778	3	24,33,33	3.37	9 (37%)	30,52,52	1.77	7 (23%)
4	PBQ	A	1780	-	17,18,18	0.72	0	19,27,27	1.32	1 (5%)

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	AD9	A	1778	3	-	0/12/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PBQ	A	1780	-	-	0/2/4/4	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1778	AD9	C4-N3	2.22	1.38	1.35
2	A	1778	AD9	C2-N3	2.23	1.36	1.32
2	A	1778	AD9	PA-O1A	2.49	1.55	1.48
2	A	1778	AD9	PB-O2B	3.51	1.56	1.48
2	A	1778	AD9	PB-O3A	4.06	1.68	1.60

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1778	AD9	O3A-PB-O1B	-4.20	98.72	108.79
2	A	1778	AD9	N3-C2-N1	-3.62	126.12	128.89
2	A	1778	AD9	O2A-PA-O3A	-2.94	100.77	108.79
2	A	1778	AD9	PA-O5'-C5'	2.59	129.17	120.25
2	A	1778	AD9	O3B-PB-O3A	2.90	106.22	100.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1778	AD9	2	0
4	A	1780	PBQ	11	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	776/788 (98%)	-0.11	48 (6%) 24 15	8, 35, 92, 96	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	765	ASN	10.7
1	A	769	MET	8.7
1	A	719	SER	7.0
1	A	762	LEU	6.8
1	A	767	PRO	6.4

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(Å ²)	Q<0.9
4	PBQ	A	1780	17/17	0.67	0.62	9.51	31,35,39,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	AD9	A	1778	31/31	0.96	0.17	0.61	13,28,36,40	0
3	MG	A	1779	1/1	0.51	0.21	-	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.