



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:10 PM GMT

PDB ID : 1SDM
Title : Crystal structure of kinesin-like calmodulin binding protein
Authors : Vinogradova, M.V.; Reddy, V.S.; Reddy, A.S.; Sablin, E.P.; Fletterick, R.J.
Deposited on : 2004-02-13
Resolution : 2.30 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 (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

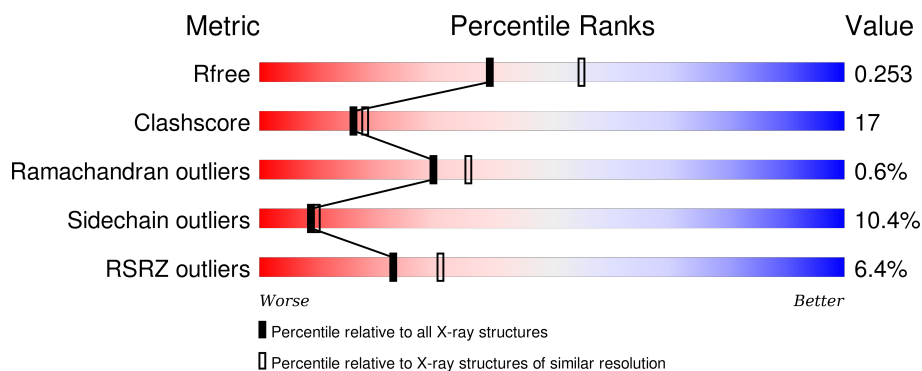
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

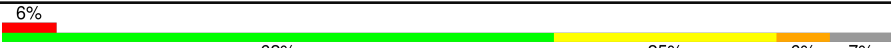
The reported resolution of this entry is 2.30 Å.

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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	369	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2860 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.

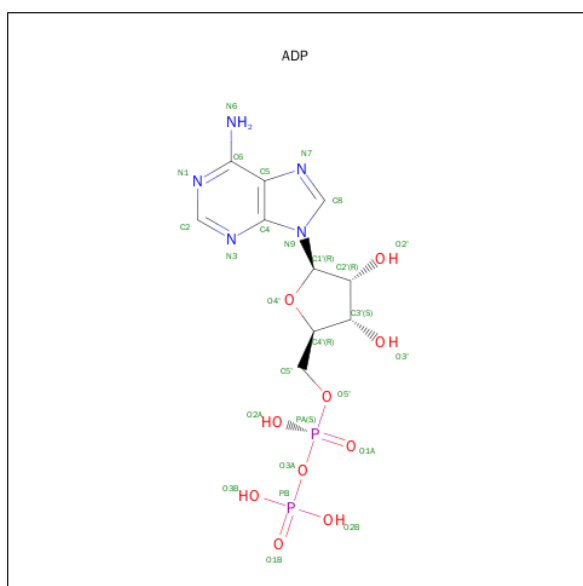
- Molecule 1 is a protein called kinesin heavy chain-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2720	1701	474	533	12			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

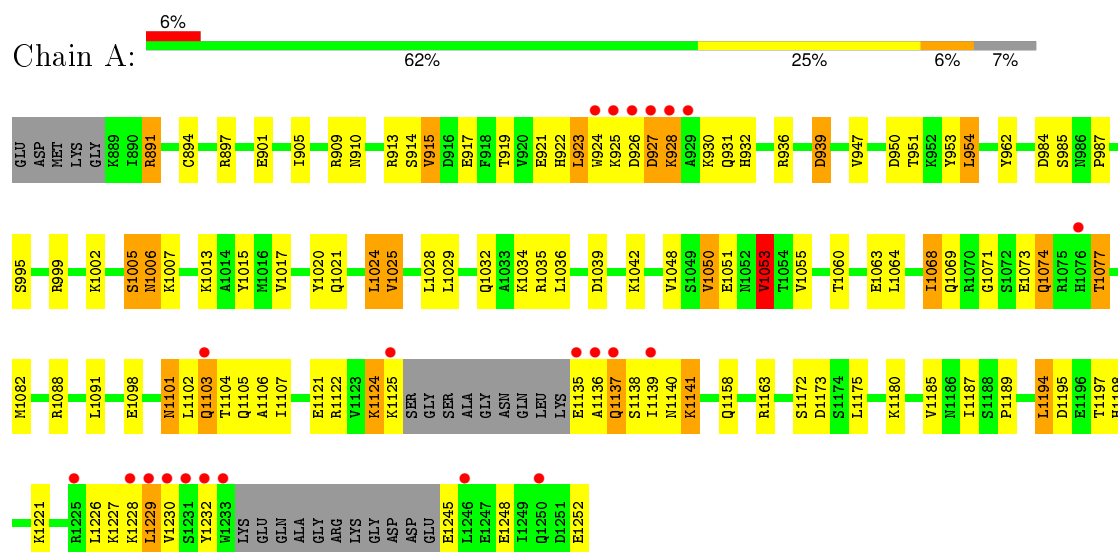
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total 112	O 112	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 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 ($\text{RSRZ} > 2$). 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: kinesin heavy chain-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.73Å 85.30Å 44.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.80 – 2.30 24.80 – 2.29	Depositor EDS
% Data completeness (in resolution range)	90.3 (24.80-2.30) 89.9 (24.80-2.29)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.03 (at 2.28Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.254 0.215 , 0.253	Depositor DCC
R_{free} test set	747 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 15282 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2860	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.38% 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, ADP

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	0.41	0/2757	0.71	0/3708

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	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1020	TYR	Sidechain
1	A	1025	VAL	Mainchain
1	A	1053	VAL	Mainchain
1	A	928	LYS	Mainchain

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	2720	0	2745	93	0
2	A	1	0	0	0	0
3	A	27	0	12	0	0
4	A	112	0	0	9	0
All	All	2860	0	2757	93	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 17.

All (93) 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:1227:LYS:O	1:A:1230:VAL:HG22	1.46	1.16
1:A:923:LEU:H	1:A:923:LEU:HD23	1.16	1.06
1:A:1139:ILE:HA	1:A:1141:LYS:HD3	1.47	0.96
1:A:1229:LEU:O	1:A:1232:TYR:HB3	1.67	0.95
1:A:913:ARG:HE	1:A:914:SER:H	1.17	0.91
1:A:1103:GLN:HG3	1:A:1104:THR:H	1.38	0.87
1:A:1017:VAL:HG23	1:A:1025:VAL:O	1.75	0.87
1:A:1103:GLN:HG3	1:A:1104:THR:N	1.91	0.85
1:A:1229:LEU:O	1:A:1232:TYR:CB	2.32	0.78
1:A:1245:GLU:HB3	4:A:100:HOH:O	1.84	0.77
1:A:932:HIS:HD2	4:A:72:HOH:O	1.71	0.72
1:A:1050:VAL:HG22	1:A:1053:VAL:HB	1.71	0.72
1:A:923:LEU:H	1:A:923:LEU:CD2	1.93	0.67
1:A:1187:ILE:HG23	1:A:1197:THR:HG23	1.77	0.67
1:A:995:SER:O	1:A:999:ARG:HD3	1.95	0.66
1:A:1032:GLN:CD	1:A:1032:GLN:H	1.99	0.65
1:A:1050:VAL:O	1:A:1050:VAL:HG22	1.95	0.65
1:A:1021:GLN:HG2	1:A:1141:LYS:HE3	1.79	0.65
1:A:923:LEU:HD23	1:A:923:LEU:N	2.02	0.63
1:A:913:ARG:NE	1:A:914:SER:H	1.94	0.63
1:A:1068:ILE:HD12	1:A:1068:ILE:O	1.98	0.63
1:A:1252:GLU:HG2	1:A:1252:GLU:OXT	1.98	0.63
1:A:924:TRP:CZ3	1:A:1194:LEU:HD22	2.33	0.62
1:A:1077:THR:HG21	4:A:19:HOH:O	1.98	0.62
1:A:1195:ASP:HB2	4:A:34:HOH:O	1.99	0.61
1:A:1106:ALA:C	1:A:1107:ILE:HD12	2.20	0.61
1:A:1135:GLU:HG3	1:A:1135:GLU:O	2.00	0.60
1:A:1226:LEU:O	1:A:1230:VAL:HG13	2.02	0.60
1:A:1021:GLN:HG2	1:A:1141:LYS:CE	2.32	0.60
1:A:1034:LYS:HE3	1:A:1036:LEU:HD21	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:TYR:CE1	1:A:954:LEU:HD13	2.37	0.59
1:A:1006:ASN:HD22	1:A:1006:ASN:H	1.49	0.59
1:A:913:ARG:NH2	1:A:939:ASP:HB2	2.18	0.59
1:A:924:TRP:CE3	1:A:1194:LEU:HD22	2.39	0.58
1:A:1101:ASN:HD22	1:A:1102:LEU:N	2.01	0.58
1:A:1060:THR:CG2	1:A:1063:GLU:HG3	2.34	0.56
1:A:1125:LYS:HB2	1:A:1137:GLN:HB3	1.88	0.56
1:A:917:GLU:HG2	1:A:936:ARG:HE	1.70	0.56
1:A:1228:LYS:O	1:A:1228:LYS:CG	2.54	0.56
1:A:915:VAL:HB	1:A:919:THR:HB	1.89	0.55
1:A:917:GLU:HG2	1:A:936:ARG:NE	2.22	0.55
1:A:1124:LYS:HA	1:A:1136:ALA:HA	1.89	0.55
1:A:909:ARG:NH2	4:A:83:HOH:O	2.40	0.54
1:A:1017:VAL:HG22	1:A:1024:LEU:HD22	1.91	0.53
1:A:922:HIS:CD2	1:A:1194:LEU:HD21	2.43	0.53
1:A:985:SER:O	1:A:987:PRO:HD3	2.09	0.53
1:A:1069:GLN:O	1:A:1073:GLU:HG3	2.09	0.53
1:A:1017:VAL:CG2	1:A:1025:VAL:O	2.54	0.52
1:A:1017:VAL:HG21	1:A:1024:LEU:HD13	1.91	0.52
1:A:1163:ARG:HH11	1:A:1248:GLU:HB3	1.76	0.50
1:A:1228:LYS:O	1:A:1228:LYS:HG2	2.11	0.49
1:A:1050:VAL:O	1:A:1050:VAL:CG2	2.59	0.48
1:A:1077:THR:HG22	4:A:18:HOH:O	2.13	0.48
1:A:1139:ILE:HG22	4:A:111:HOH:O	2.14	0.48
1:A:1060:THR:HG22	1:A:1063:GLU:OE1	2.13	0.48
1:A:1101:ASN:HD22	1:A:1101:ASN:C	2.17	0.48
1:A:1141:LYS:HG2	4:A:30:HOH:O	2.13	0.47
1:A:1032:GLN:N	1:A:1032:GLN:CD	2.66	0.47
1:A:901:GLU:O	1:A:905:ILE:HG12	2.14	0.47
1:A:930:LYS:NZ	1:A:1198:HIS:HE1	2.12	0.47
1:A:923:LEU:HG	1:A:923:LEU:O	2.14	0.46
1:A:921:GLU:HB2	1:A:931:GLN:HG2	1.96	0.46
1:A:947:VAL:O	1:A:951:THR:HG23	2.15	0.46
1:A:962:TYR:CE1	1:A:1180:LYS:HE3	2.51	0.46
1:A:1138:SER:O	4:A:111:HOH:O	2.20	0.46
1:A:1125:LYS:HB2	1:A:1137:GLN:CB	2.45	0.46
1:A:1137:GLN:O	1:A:1137:GLN:HG3	2.11	0.46
1:A:1187:ILE:CG2	1:A:1197:THR:HG23	2.45	0.45
1:A:1060:THR:HG23	1:A:1063:GLU:HG3	1.98	0.45
1:A:897:ARG:O	1:A:1189:PRO:HG3	2.15	0.45
1:A:1229:LEU:HD23	1:A:1229:LEU:HA	1.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:VAL:O	1:A:1185:VAL:HG13	2.17	0.45
1:A:1048:VAL:HG11	1:A:1172:SER:HB2	1.99	0.44
1:A:924:TRP:HZ3	1:A:1194:LEU:HD22	1.81	0.44
1:A:1007:LYS:O	1:A:1102:LEU:HG	2.18	0.44
1:A:1107:ILE:N	1:A:1107:ILE:HD12	2.32	0.44
1:A:926:ASP:HB3	1:A:927:ASP:H	1.53	0.44
1:A:1015:TYR:HA	1:A:1028:LEU:HD12	2.00	0.44
1:A:1105:GLN:HB3	1:A:1221:LYS:HG2	1.99	0.43
1:A:1039:ASP:O	1:A:1050:VAL:HA	2.18	0.43
1:A:1048:VAL:HG22	1:A:1173:ASP:OD2	2.19	0.43
1:A:1122:ARG:HG3	1:A:1140:ASN:ND2	2.33	0.43
1:A:1071:GLY:O	1:A:1074:GLN:HB3	2.19	0.43
1:A:1002:LYS:O	1:A:1005:SER:HB2	2.19	0.42
1:A:1013:LYS:HE2	1:A:1055:VAL:HG11	2.01	0.42
1:A:1082:MET:CE	1:A:1121:GLU:HG3	2.50	0.42
1:A:1029:LEU:CD2	1:A:1035:ARG:HB3	2.50	0.42
1:A:891:ARG:HH11	1:A:891:ARG:HG3	1.85	0.42
1:A:894:CYS:HA	1:A:1185:VAL:CG1	2.50	0.41
1:A:923:LEU:CD2	1:A:923:LEU:N	2.70	0.41
1:A:1048:VAL:CG1	1:A:1172:SER:HB2	2.50	0.41
1:A:922:HIS:CD2	1:A:924:TRP:HB2	2.56	0.40
1:A:1124:LYS:HB2	1:A:1135:GLU:O	2.21	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	338/369 (92%)	324 (96%)	12 (4%)	2 (1%)	30 36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	927	ASP
1	A	915	VAL

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	308/326 (94%)	276 (90%)	32 (10%)	9 10

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	891	ARG
1	A	910	ASN
1	A	923	LEU
1	A	925	LYS
1	A	928	LYS
1	A	939	ASP
1	A	950	ASP
1	A	954	LEU
1	A	984	ASP
1	A	1005	SER
1	A	1006	ASN
1	A	1024	LEU
1	A	1042	LYS
1	A	1050	VAL
1	A	1051	GLU
1	A	1053	VAL
1	A	1064	LEU
1	A	1068	ILE
1	A	1074	GLN
1	A	1077	THR
1	A	1088	ARG
1	A	1091	LEU
1	A	1098	GLU
1	A	1101	ASN
1	A	1103	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1124	LYS
1	A	1137	GLN
1	A	1141	LYS
1	A	1158	GLN
1	A	1175	LEU
1	A	1194	LEU
1	A	1229	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	922	HIS
1	A	931	GLN
1	A	1006	ASN
1	A	1021	GLN
1	A	1052	ASN
1	A	1074	GLN
1	A	1101	ASN
1	A	1103	GLN
1	A	1157	ASN
1	A	1158	GLN
1	A	1198	HIS

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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	ADP	A	600	2	22,29,29	1.09	1 (4%)	27,45,45	1.86	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
3	ADP	A	600	2	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	ADP	C2-N1	3.06	1.39	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	ADP	N3-C2-N1	-7.42	123.21	128.89
3	A	600	ADP	C2-N1-C6	2.66	123.52	118.77
3	A	600	ADP	C4'-O4'-C1'	2.88	112.89	109.72

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 [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	344/369 (93%)	0.24	22 (6%)	23 31	14, 31, 60, 61	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1137	GLN	6.8
1	A	927	ASP	6.5
1	A	1225	ARG	5.2
1	A	926	ASP	4.8
1	A	1250	GLN	4.8
1	A	1231	SER	4.8
1	A	1125	LYS	4.7
1	A	1233	TRP	4.5
1	A	929	ALA	4.0
1	A	1136	ALA	4.0
1	A	1232	TYR	4.0
1	A	1228	LYS	3.8
1	A	928	LYS	3.8
1	A	1229	LEU	3.3
1	A	1076	HIS	3.2
1	A	1230	VAL	3.1
1	A	1135	GLU	3.0
1	A	925	LYS	2.7
1	A	1103	GLN	2.5
1	A	924	TRP	2.4
1	A	1246	LEU	2.4
1	A	1139	ILE	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, 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
3	ADP	A	600	27/27	0.97	0.10	-0.48	16,28,33,37	0
2	MG	A	601	1/1	0.98	0.08	-	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.