



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2018 – 02:43 am GMT

PDB ID : 1R6B
Title : High resolution crystal structure of ClpA
Authors : Xia, D.; Maurizi, M.R.; Guo, F.; Singh, S.K.; Esser, L.
Deposited on : 2003-10-15
Resolution : 2.25 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

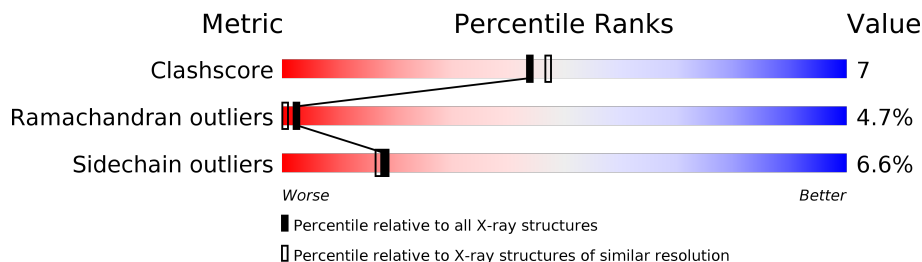
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	122078	1286 (2.26-2.26)
Ramachandran outliers	120005	1253 (2.26-2.26)
Sidechain outliers	119972	1254 (2.26-2.26)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	X	758	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5623 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 ClpA protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	704	Total	C	N	O	S	0	0	0
			5506	3466	986	1037	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	169	LEU	MET	ENGINEERED	UNP P0ABH9
X	367	ALA	GLY	SEE REMARK 999	UNP P0ABH9
X	411	LEU	VAL	SEE REMARK 999	UNP P0ABH9
X	533	LEU	VAL	SEE REMARK 999	UNP P0ABH9

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	3	Total	Mg	0	0
			3	3		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is water.

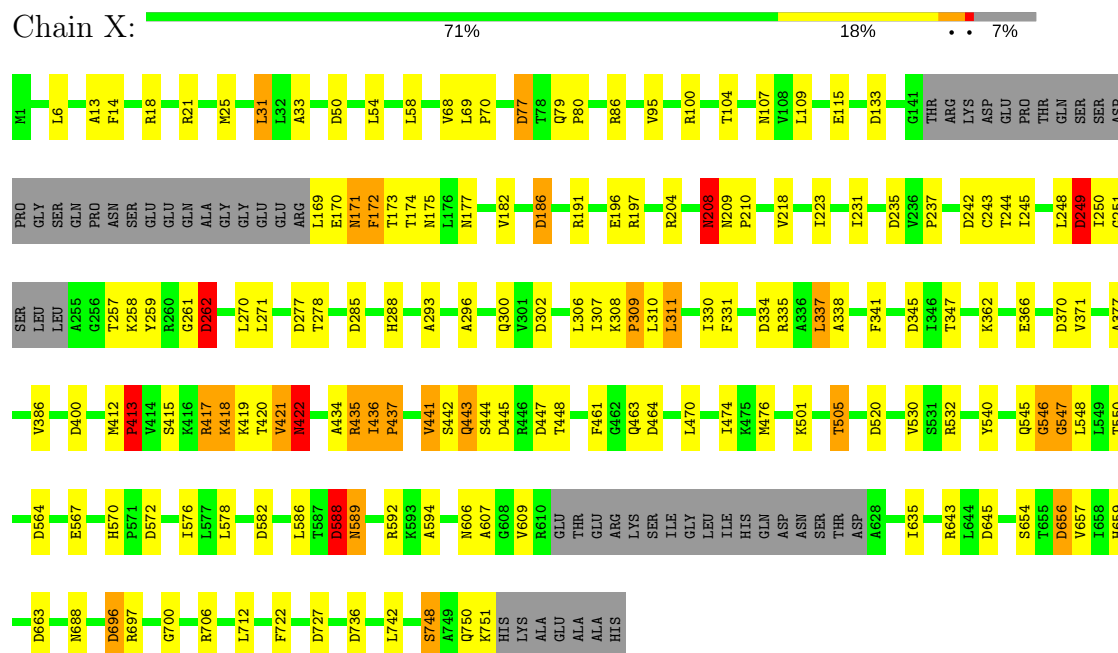
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	X	60	Total O 60 60	0	0

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.

Note EDS was not executed.

- Molecule 1: ClpA protein



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	124.11Å 124.11Å 97.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.25	Depositor
% Data completeness (in resolution range)	93.8 (20.00-2.25)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.234 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5623	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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: 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	X	0.76	4/5586 (0.1%)	0.72	28/7540 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	218	VAL	CB-CG1	-7.11	1.38	1.52
1	X	422	ASN	CB-CG	-6.06	1.37	1.51
1	X	386	VAL	CB-CG2	-5.76	1.40	1.52
1	X	208	ASN	CB-CG	-5.19	1.39	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	588	ASP	CB-CG-OD2	5.87	123.58	118.30
1	X	133	ASP	CB-CG-OD2	5.69	123.42	118.30
1	X	736	ASP	CB-CG-OD2	5.53	123.28	118.30
1	X	663	ASP	CB-CG-OD2	5.50	123.25	118.30
1	X	262	ASP	CB-CG-OD2	5.48	123.23	118.30
1	X	77	ASP	CB-CG-OD2	5.44	123.20	118.30
1	X	249	ASP	CB-CG-OD2	5.43	123.19	118.30
1	X	696	ASP	CB-CG-OD2	5.40	123.16	118.30
1	X	445	ASP	CB-CG-OD2	5.38	123.14	118.30
1	X	520	ASP	CB-CG-OD2	5.33	123.09	118.30
1	X	727	ASP	CB-CG-OD2	5.31	123.08	118.30
1	X	334	ASP	CB-CG-OD2	5.30	123.07	118.30
1	X	235	ASP	CB-CG-OD2	5.30	123.07	118.30
1	X	447	ASP	CB-CG-OD2	5.29	123.06	118.30
1	X	564	ASP	CB-CG-OD2	5.24	123.02	118.30
1	X	50	ASP	CB-CG-OD2	5.24	123.02	118.30
1	X	370	ASP	CB-CG-OD2	5.23	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	582	ASP	CB-CG-OD2	5.21	122.99	118.30
1	X	645	ASP	CB-CG-OD2	5.21	122.99	118.30
1	X	400	ASP	CB-CG-OD2	5.21	122.99	118.30
1	X	186	ASP	CB-CG-OD2	5.19	122.97	118.30
1	X	345	ASP	CB-CG-OD2	5.18	122.96	118.30
1	X	464	ASP	CB-CG-OD2	5.17	122.95	118.30
1	X	302	ASP	CB-CG-OD2	5.16	122.94	118.30
1	X	656	ASP	CB-CG-OD2	5.15	122.94	118.30
1	X	242	ASP	CB-CG-OD2	5.15	122.93	118.30
1	X	277	ASP	CB-CG-OD2	5.09	122.88	118.30
1	X	285	ASP	CB-CG-OD2	5.08	122.88	118.30

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	X	5506	0	5598	80	0
2	X	3	0	0	0	0
3	X	54	0	23	0	0
4	X	60	0	0	2	0
All	All	5623	0	5621	80	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 7.

All (80) 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:X:442:SER:O	1:X:443:GLN:CG	1.77	1.32
1:X:420:THR:O	1:X:421:VAL:HG23	1.08	1.24
1:X:420:THR:O	1:X:421:VAL:CG2	1.94	1.16
1:X:442:SER:O	1:X:443:GLN:HG3	0.85	1.02
1:X:550:THR:HG23	1:X:594:ALA:HB2	1.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:436:ILE:H	1:X:437:PRO:CD	1.82	0.93
1:X:250:ILE:HG22	1:X:251:GLY:H	1.41	0.86
1:X:442:SER:C	1:X:443:GLN:HG3	1.96	0.85
1:X:104:THR:H	1:X:107:ASN:HD22	1.27	0.81
1:X:436:ILE:H	1:X:437:PRO:HD2	1.43	0.81
1:X:420:THR:C	1:X:421:VAL:HG23	2.02	0.80
1:X:377:ALA:HB2	1:X:422:ASN:HB3	1.66	0.78
1:X:434:ALA:O	1:X:435:ARG:HB2	1.87	0.74
1:X:250:ILE:HG22	1:X:251:GLY:N	2.04	0.72
1:X:607:ALA:HB1	1:X:635:ILE:HD13	1.72	0.70
1:X:418:LYS:HD3	1:X:422:ASN:OD1	1.94	0.67
1:X:418:LYS:HE2	1:X:422:ASN:HD21	1.63	0.64
1:X:436:ILE:N	1:X:437:PRO:CD	2.59	0.63
1:X:177:ASN:ND2	1:X:245:ILE:H	1.95	0.63
1:X:13:ALA:HB2	1:X:33:ALA:HB2	1.80	0.62
1:X:191:ARG:HD3	1:X:223:ILE:HD11	1.82	0.62
1:X:169:LEU:HD12	1:X:170:GLU:H	1.65	0.62
1:X:261:GLY:O	1:X:262:ASP:HB2	1.99	0.61
1:X:69:LEU:N	1:X:70:PRO:HD3	2.14	0.61
1:X:271:LEU:HD13	1:X:307:ILE:HG13	1.83	0.61
1:X:442:SER:O	1:X:443:GLN:CB	2.49	0.60
1:X:589:ASN:HB3	1:X:592:ARG:HD2	1.83	0.60
1:X:250:ILE:CG2	1:X:251:GLY:H	2.11	0.60
1:X:171:ASN:O	1:X:172:PHE:HB2	2.01	0.60
1:X:436:ILE:N	1:X:437:PRO:HD2	2.15	0.60
1:X:550:THR:HG21	1:X:588:ASP:OD1	2.02	0.60
1:X:546:GLY:O	1:X:589:ASN:ND2	2.35	0.59
1:X:14:PHE:O	1:X:18:ARG:HG3	2.03	0.59
1:X:337:LEU:HD12	1:X:341:PHE:HE1	1.69	0.57
1:X:417:ARG:O	1:X:418:LYS:HB2	2.04	0.57
1:X:570:HIS:HD2	1:X:572:ASP:HB2	1.71	0.55
1:X:204:ARG:O	1:X:208:ASN:ND2	2.38	0.55
1:X:659:HIS:CE1	1:X:688:ASN:HD22	2.25	0.54
1:X:249:ASP:N	1:X:249:ASP:OD1	2.41	0.54
1:X:31:LEU:HD13	1:X:58:LEU:HD11	1.90	0.53
1:X:308:LYS:HB2	1:X:309:PRO:HD3	1.93	0.51
1:X:68:VAL:HG12	1:X:70:PRO:HD3	1.92	0.51
1:X:191:ARG:NH1	4:X:901:HOH:O	2.43	0.51
1:X:306:LEU:HD23	1:X:311:LEU:HD13	1.92	0.50
1:X:545:GLN:O	1:X:547:GLY:N	2.45	0.50
1:X:578:LEU:HD22	1:X:643:ARG:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:371:VAL:HG22	1:X:418:LYS:HD2	1.95	0.48
1:X:436:ILE:H	1:X:437:PRO:HD3	1.71	0.48
1:X:659:HIS:CE1	1:X:688:ASN:ND2	2.82	0.47
1:X:588:ASP:CG	1:X:589:ASN:N	2.66	0.47
1:X:659:HIS:HE1	1:X:688:ASN:ND2	2.13	0.47
1:X:309:PRO:HB2	1:X:310:LEU:H	1.58	0.46
1:X:25:MET:HB3	1:X:80:PRO:HA	1.97	0.46
1:X:288:HIS:HB2	1:X:330:ILE:HD11	1.98	0.45
1:X:308:LYS:HE3	1:X:337:LEU:HD13	1.97	0.45
1:X:337:LEU:HD12	1:X:341:PHE:CE1	2.49	0.45
1:X:86:ARG:NH1	1:X:115:GLU:OE2	2.50	0.45
1:X:748:SER:C	1:X:750:GLN:H	2.20	0.45
1:X:570:HIS:CD2	1:X:572:ASP:H	2.35	0.44
1:X:191:ARG:NH2	1:X:347:THR:O	2.50	0.44
1:X:197:ARG:HD3	4:X:941:HOH:O	2.18	0.44
1:X:169:LEU:HD23	1:X:174:THR:HG23	2.01	0.43
1:X:588:ASP:OD1	1:X:588:ASP:C	2.58	0.43
1:X:362:LYS:HD3	1:X:366:GLU:OE2	2.19	0.42
1:X:412:MET:O	1:X:413:PRO:C	2.57	0.42
1:X:95:VAL:HG13	1:X:100:ARG:HB2	2.00	0.42
1:X:540:TYR:HA	1:X:540:TYR:HD2	1.71	0.42
1:X:589:ASN:CB	1:X:592:ARG:HD2	2.49	0.42
1:X:209:ASN:HA	1:X:210:PRO:HD3	1.90	0.42
1:X:434:ALA:O	1:X:435:ARG:CB	2.64	0.42
1:X:79:GLN:HA	1:X:80:PRO:HD3	1.92	0.42
1:X:169:LEU:HB3	1:X:174:THR:HG21	2.01	0.42
1:X:501:LYS:O	1:X:505:THR:HG23	2.20	0.41
1:X:177:ASN:HD21	1:X:245:ILE:H	1.68	0.41
1:X:576:ILE:HG23	1:X:586:LEU:HD21	2.02	0.41
1:X:250:ILE:CG2	1:X:251:GLY:N	2.72	0.40
1:X:470:LEU:O	1:X:474:ILE:HG12	2.21	0.40
1:X:231:ILE:HG21	1:X:243:CYS:O	2.21	0.40
1:X:461:PHE:HB2	1:X:657:VAL:HG13	2.03	0.40
1:X:696:ASP:O	1:X:700:GLY:N	2.51	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	X	696/758 (92%)	604 (87%)	59 (8%)	33 (5%)	2 0

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	171	ASN
1	X	172	PHE
1	X	262	ASP
1	X	413	PRO
1	X	415	SER
1	X	417	ARG
1	X	421	VAL
1	X	435	ARG
1	X	436	ILE
1	X	443	GLN
1	X	175	ASN
1	X	296	ALA
1	X	300	GLN
1	X	309	PRO
1	X	418	LYS
1	X	419	LYS
1	X	422	ASN
1	X	437	PRO
1	X	546	GLY
1	X	548	LEU
1	X	293	ALA
1	X	335	ARG
1	X	441	VAL
1	X	258	LYS
1	X	444	SER
1	X	530	VAL
1	X	532	ARG
1	X	173	THR

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Mol	Chain	Res	Type
1	X	237	PRO
1	X	338	ALA
1	X	609	VAL
1	X	182	VAL
1	X	547	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	X	592/639 (93%)	553 (93%)	39 (7%)	18	17

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	6	LEU
1	X	21	ARG
1	X	31	LEU
1	X	54	LEU
1	X	77	ASP
1	X	109	LEU
1	X	186	ASP
1	X	196	GLU
1	X	208	ASN
1	X	244	THR
1	X	248	LEU
1	X	249	ASP
1	X	257	THR
1	X	259	TYR
1	X	270	LEU
1	X	278	THR
1	X	311	LEU
1	X	331	PHE
1	X	337	LEU
1	X	413	PRO
1	X	422	ASN

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Mol	Chain	Res	Type
1	X	441	VAL
1	X	448	THR
1	X	463	GLN
1	X	476	MET
1	X	505	THR
1	X	567	GLU
1	X	588	ASP
1	X	589	ASN
1	X	606	ASN
1	X	654	SER
1	X	656	ASP
1	X	697	ARG
1	X	706	ARG
1	X	712	LEU
1	X	722	PHE
1	X	742	LEU
1	X	748	SER
1	X	751	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	22	HIS
1	X	107	ASN
1	X	116	GLN
1	X	177	ASN
1	X	200	GLN
1	X	422	ASN
1	X	483	HIS
1	X	570	HIS
1	X	606	ASN
1	X	659	HIS
1	X	660	GLN
1	X	688	ASN

5.3.3 RNA ⓘ

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 5 ligands modelled in this entry, 3 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	ADP	X	780	2	25,29,29	1.37	4 (16%)	25,45,45	2.14	4 (16%)
3	ADP	X	781	2	25,29,29	1.26	3 (12%)	25,45,45	2.20	2 (8%)

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	X	780	2	-	0/12/32/32	0/3/3/3
3	ADP	X	781	2	-	0/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	780	ADP	O3'-C3'	-3.43	1.34	1.43
3	X	780	ADP	C2'-C3'	-2.34	1.47	1.53
3	X	780	ADP	O2'-C2'	-2.02	1.38	1.43
3	X	780	ADP	C4-N3	-2.01	1.32	1.35
3	X	781	ADP	O4'-C1'	2.01	1.44	1.41
3	X	781	ADP	C2-N1	2.49	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	781	ADP	C2-N3	3.12	1.37	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	781	ADP	N3-C2-N1	-9.94	120.36	128.86
3	X	780	ADP	N3-C2-N1	-9.29	120.91	128.86
3	X	780	ADP	PA-O3A-PB	-3.08	122.29	132.63
3	X	780	ADP	O3'-C3'-C2'	-2.36	104.27	111.83
3	X	780	ADP	O3'-C3'-C4'	-2.34	104.28	111.06
3	X	781	ADP	PA-O3A-PB	-2.21	125.22	132.63

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 [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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.