



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 03:10 pm GMT

PDB ID : 2V7Z
Title : CRYSTAL STRUCTURE OF THE 70-KDA HEAT SHOCK COGNATE PROTEIN FROM RATTUS NORVEGICUS IN POST-ATP HYDROLYSIS STATE
Authors : Chang, Y.-W.; Sun, Y.-J.; Wang, C.; Hsiao, C.-D.
Deposited on : 2007-08-02
Resolution : 3.50 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
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) : recalc28949

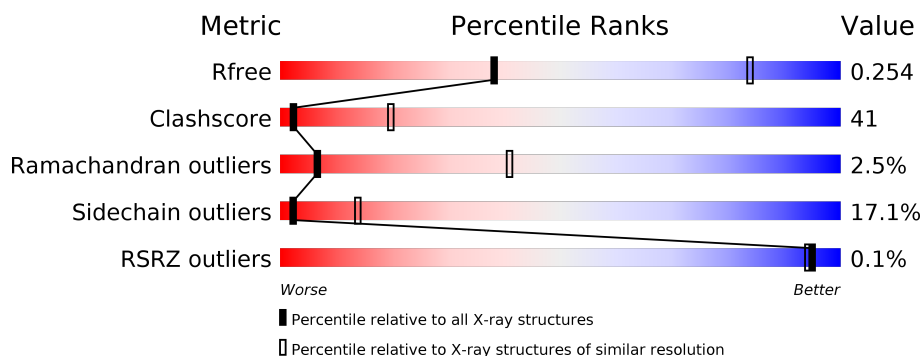
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
R_{free}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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	543	
1	B	543	

2 Entry composition [i](#)

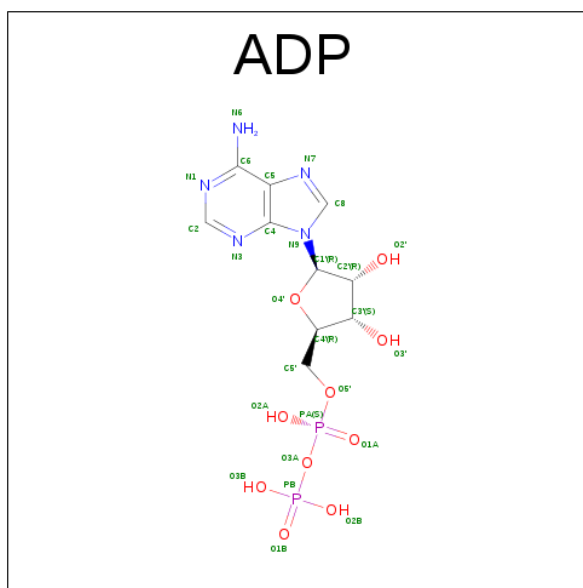
There are 4 unique types of molecules in this entry. The entry contains 6062 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HEAT SHOCK COGNATE 71 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	1
			2952	1851	522	571	8			
1	B	382	Total	C	N	O	S	0	0	1
			2952	1851	522	571	8			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

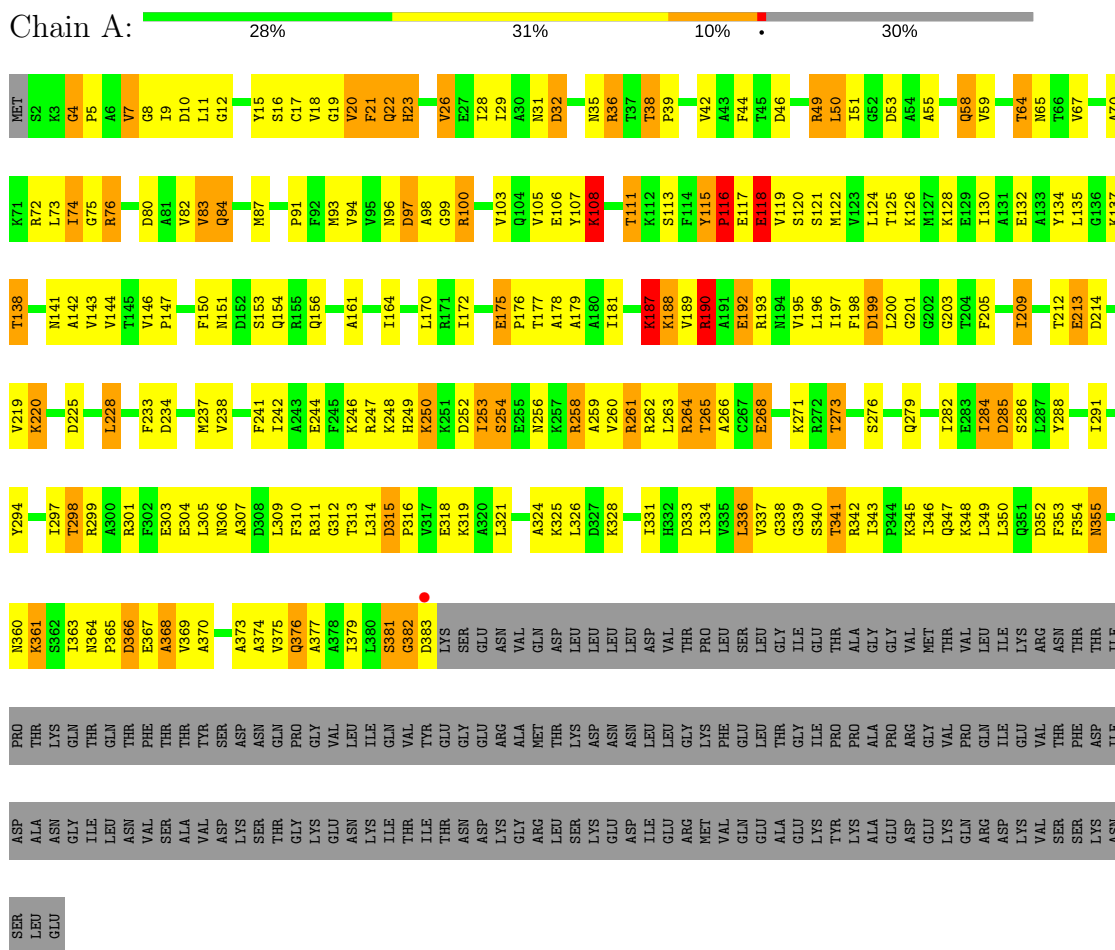
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	51	Total	O	0	0
			51	51		
4	B	43	Total	O	0	0
			43	43		

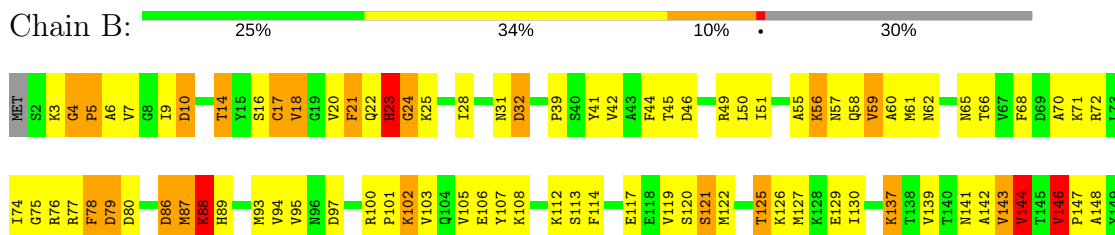
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: HEAT SHOCK COGNATE 71 KDA PROTEIN



• Molecule 1: HEAT SHOCK COGNATE 71 KDA PROTEIN



Lys	ASP	K357	T295	F150
	ILE	E358	S296	N151
	ASP	L359	I297	D152
	ALA	K360	T298	S153
	ASN	K361	R299	Q154
	GLY	S362	A300	Q155
	ILE	L363	R301	
	LEU	N364	F302	K159
	ASN	P365	E303	A161
	VAL	D366	E304	G162
Ser	SER	E367	L305	G163
	ALA	A368	N306	T163
	VAL	P369	A307	N235
	ASP	A370	D308	R236
	LYS	P371	L309	M237
	SER	G372	F310	V238
	THR	A373	R311	N239
	GLN		G312	H240
	PRO		L313	F241
	LYS	Q376	L314	I242
Glu	GLU	A377	L314	I243
	ASN	A378	D315	A243
	ILE		P316	K246
	LYS		V317	R247
	ILE	S381	E318	K248
	THR	VAL	K319	H249
	ILE	D383	A320	K250
	THR	GLY	L321	K251
	ASN	SER	G322	K252
	ASP	GLU	R323	I253
Lys	LYS	ASN	D323	
	GLY	VAL	A324	K185
	ARG	GLN	K325	
	MET	THR	L326	K188
	LEU	ASP	D327	V189
	LYS	LYS	K328	R190
	LYS	ASP	LEU	A191
	GLU	ASN	LEU	E192
	ASP	ASN	ASP	R193
	ILE	LEU	GLY	N194
Glu	GLU	VAL	D333	V195
	ARG	GLY	L334	
	MET	PRO	V335	L196
	VAL	LYS	L336	I197
	GLN	GLU	P337	F198
	GLU	LEU	G338	D199
	ALA	THR	G339	L200
	GLU	ILE	S340	Z201
	LYS	ILE	GLU	G202
	TYR	PRO	THR	A280
Lys	PRO	ALA	I343	K281
	ALA	GLY	P344	D206
	GLU	PRO	K345	F207
	ASP	ARG	L346	S208
	GLU	GLY	Q347	L209
	LYS	VAL	MET	D285
	VAL	THR	K348	L210
	GLN	PRO	L349	S286
	ARG	GLN	L350	L287
	ASP	ILE	LEU	Y288
Val	LYS	ILE	Q351	T212
	GLU	GLY	D352	E213
	VAL	VAL	K353	D214
	VAL	ARG	F354	G215
	SER	ASN	N355	I216
	THR	THR	G356	F217
	DUR			

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	179.85Å 94.79Å 78.23Å 90.00° 93.24° 90.00°	Depositor
Resolution (Å)	29.01 – 3.50 29.01 – 3.45	Depositor EDS
% Data completeness (in resolution range)	90.7 (29.01-3.50) 87.7 (29.01-3.45)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 3.47Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.257 , 0.279 0.234 , 0.254	Depositor DCC
R_{free} test set	747 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	1.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6062	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.69	1/2997 (0.0%)	1.19	19/4046 (0.5%)
1	B	0.72	3/2998 (0.1%)	1.23	39/4048 (1.0%)
All	All	0.71	4/5995 (0.1%)	1.21	58/8094 (0.7%)

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	1	6
1	B	1	9
All	All	2	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	GLY	C-N	8.77	1.50	1.34
1	B	345	LYS	C-O	8.63	1.39	1.23
1	B	345	LYS	C-N	5.95	1.47	1.34
1	B	343	ILE	C-N	5.38	1.44	1.34

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	LYS	O-C-N	-12.45	102.78	122.70
1	B	24	GLY	O-C-N	10.98	140.26	122.70
1	B	24	GLY	CA-C-N	-10.41	94.30	117.20
1	B	344	PRO	C-N-CA	-10.25	96.08	121.70
1	B	87	MET	C-N-CA	-10.22	96.16	121.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	250	LYS	CA
1	B	199	ASP	CA

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	TYR	Mainchain
1	A	116	PRO	Mainchain
1	A	187	LYS	Mainchain
1	A	22	GLN	Mainchain
1	A	36	ARG	Mainchain

5.2 Too-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 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	2952	0	2958	246	4
1	B	2952	0	2958	253	4
2	A	27	0	12	1	0
2	B	27	0	12	2	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	51	0	0	3	0
4	B	43	0	0	6	0
All	All	6062	0	5940	494	4

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 41.

The worst 5 of 494 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:B:141:ASN:ND2	1:B:170:LEU:HD21	1.34	1.41
1:B:211:THR:O	1:B:211:THR:HG22	1.39	1.19
1:A:74:ILE:HD13	1:A:116:PRO:HB2	1.30	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:PHE:HB2	1:A:26:VAL:HA	1.29	1.09
1:A:94:VAL:HG22	1:A:103:VAL:HG12	1.37	1.06

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASN:ND2	1:B:355:ASN:OD1[4_546]	1.19	1.01
1:A:355:ASN:CG	1:B:355:ASN:OD1[4_546]	1.60	0.60
1:A:355:ASN:OD1	1:B:355:ASN:OD1[4_546]	1.85	0.35
1:A:355:ASN:ND2	1:B:355:ASN:CG[4_546]	1.96	0.24

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	379/543 (70%)	329 (87%)	39 (10%)	11 (3%)	5	38
1	B	380/543 (70%)	326 (86%)	46 (12%)	8 (2%)	8	45
All	All	759/1086 (70%)	655 (86%)	85 (11%)	19 (2%)	6	41

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	SER
1	A	368	ALA
1	A	4	GLY
1	A	23	HIS
1	A	59	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	315/459 (69%)	263 (84%)	52 (16%)	2	15
1	B	315/459 (69%)	259 (82%)	56 (18%)	2	12
All	All	630/918 (69%)	522 (83%)	108 (17%)	2	14

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	ILE
1	B	79	ASP
1	B	334	ILE
1	A	376	GLN
1	B	17	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	GLN
1	B	22	GLN
1	B	279	GLN
1	A	306	ASN
1	B	249	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

4 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	ADP	A	1383	-	25,29,29	1.40	2 (8%)	24,45,45	1.93	5 (20%)
3	PO4	A	1384	-	4,4,4	1.25	1 (25%)	6,6,6	1.39	1 (16%)
2	ADP	B	1383	-	25,29,29	1.54	3 (12%)	24,45,45	2.00	1 (4%)
3	PO4	B	1384	-	4,4,4	1.14	1 (25%)	6,6,6	1.27	0

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	ADP	A	1383	-	-	0/12/32/32	0/3/3/3
3	PO4	A	1384	-	-	0/0/0/0	0/0/0/0
2	ADP	B	1383	-	-	0/12/32/32	0/3/3/3
3	PO4	B	1384	-	-	0/0/0/0	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1384	PO4	P-O3	-2.18	1.46	1.54
3	B	1384	PO4	P-O3	-2.06	1.47	1.54
2	B	1383	ADP	C2'-C1'	2.31	1.57	1.53
2	A	1383	ADP	C5-C4	2.55	1.46	1.40
2	B	1383	ADP	C5-C4	2.68	1.46	1.40

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1383	ADP	N3-C2-N1	-7.66	122.19	128.86
2	A	1383	ADP	N3-C2-N1	-6.85	122.89	128.86
2	A	1383	ADP	C4-C5-N7	-3.02	106.50	109.41
3	A	1384	PO4	O4-P-O1	-2.34	101.02	110.97
2	A	1383	ADP	C5'-C4'-C3'	-2.21	106.87	115.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1383	ADP	1	0
2	B	1383	ADP	2	0
3	B	1384	PO4	1	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	382/543 (70%)	-0.47	1 (0%) 93 90	20, 67, 119, 163	0
1	B	382/543 (70%)	-0.47	0 100 100	14, 68, 112, 147	0
All	All	764/1086 (70%)	-0.47	1 (0%) 95 94	14, 68, 116, 163	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	383	ASP	4.1

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(Å ²)	Q<0.9
2	ADP	A	1383	27/27	0.95	0.21	0.34	77,77,77,77	0
2	ADP	B	1383	27/27	0.96	0.18	-0.29	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PO4	A	1384	5/5	0.96	0.17	-0.82	74,101,101,101	0
3	PO4	B	1384	5/5	0.98	0.11	-2.87	37,37,37,165	0

6.5 Other polymers [i](#)

There are no such residues in this entry.