



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 5, 2023 – 01:27 am 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

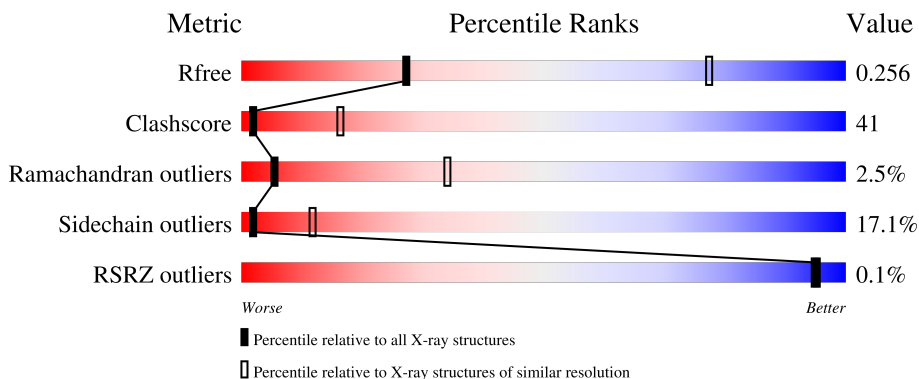
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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
			Total	C	N	O	S			
1	A	382	Total 2952	C 1851	N 522	O 571	S 8	0	0	1
1	B	382	Total 2952	C 1851	N 522	O 571	S 8	0	0	1

- 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
			Total	C	N	O	P		
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

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



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

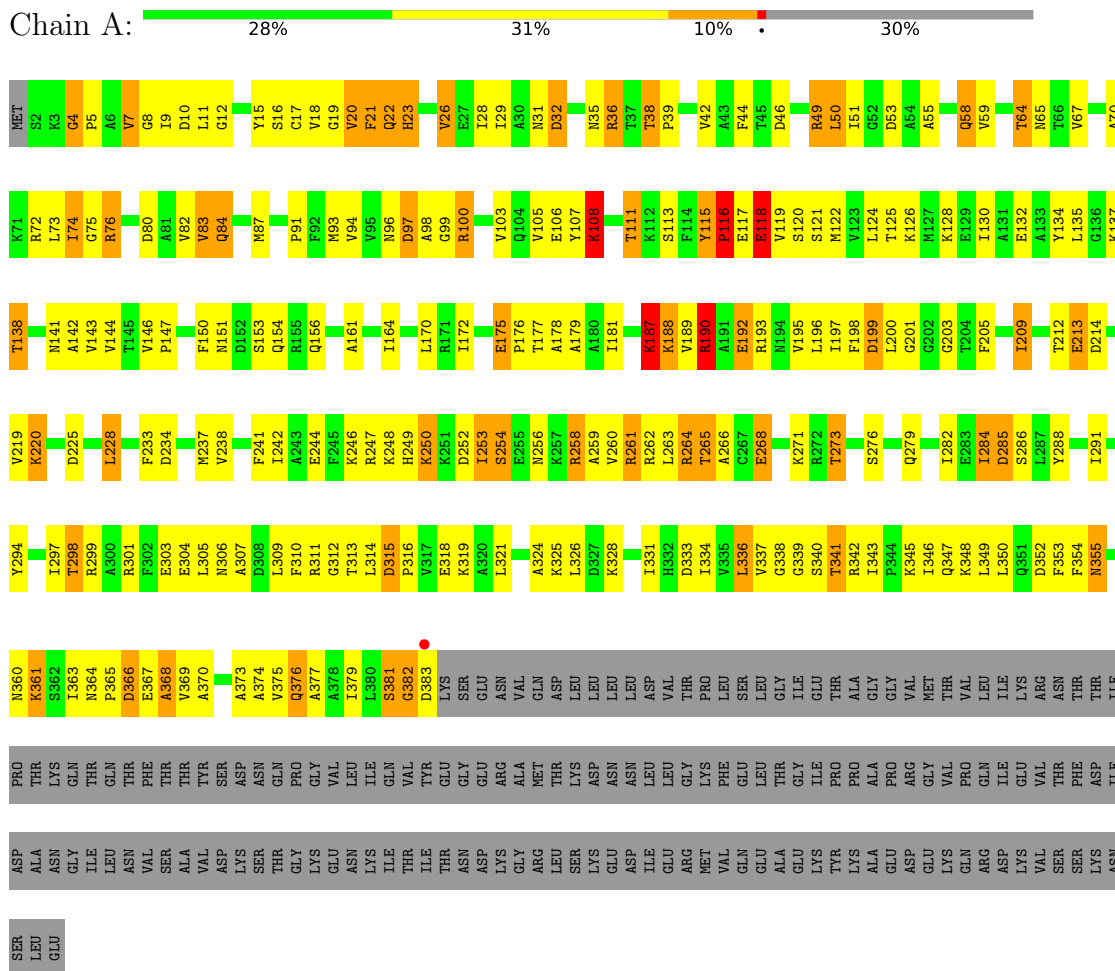
- Molecule 4 is water.

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

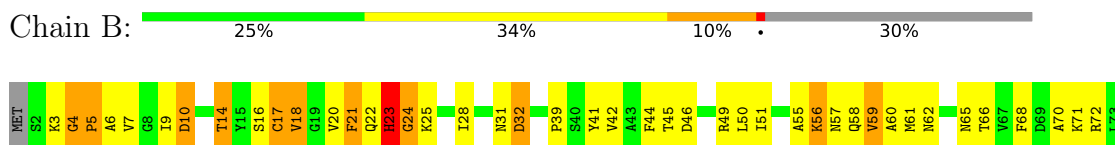
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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	THR	K357	T298	R220	F150	I74
ASN	ILE	E388	S296	K220	M151	G75
SER	ASP	L359	I297	S221	R152	R76
LEU	ALA	N360	T298	S153	S153	R77
GLU	ASN	K361	R299	A223	Q154	F78
	GLY	S362	A300	L228	D79	D80
	ILE	I363	R301	G229	K159	
	LEU	N364	F302	D86	D160	
	LEU	N365	E303	A161	A161	M87
	ASN	D366	E304	G162	K88	K89
	VAL	E367	L305	L163	H89	
	ALA	A368	N306	R236	M83	
	VAL	V369	A307	M237	V94	
	ASP	A370	D308	V238	V169	
	ASP	Y371	L309	N239	L170	
	LYS	G372	F310	H240	N96	
	SER	A373	R311	F241	R171	
	THR		G312	I242	I172	
	THR		T313	A243	I173	
	GLY		L314	K246	M174	
	GLU		D315	R247	E175	
	VAL		A378	K248	P176	
	ASN		P316	K249	T177	
	LEU		V317	H249	A178	
	ILE		E318	K250	E179	
	THR		K319	R251	I107	
	GLU		A320	I253	K108	
	ASN		L321	K257	K112	
	ASN		R322		S113	
	GLU		D323	R261	F114	
	LYS		A324	R262	E117	
	GLY		K325	L263	E118	
	ARG		L326	R264	V119	
	LEU		D327	E268	S120	
	THR		K328	R269	S121	
	ASP		I331	T273	M122	
	LEU		H332	L274	T125	
	LEU		D333		K126	
	LEU		I334		F198	
	GLY		V335		D199	
	ARG		L336		M127	
	MET		V337		K128	
	VAL		V338		E129	
	VAL		G338		I130	
	GLN		G339		K137	
	GLU		S340		T138	
	ALA		I343		V139	
	GLY		P344		T140	
	LYS		K345		A142	
	PRO		I346		V143	
	ARG		Q347		V144	
	GLY		K348		T145	
	PRO		L349		K146	
	ASP		L350		P147	
	ASP		V351		A148	
	GLU		G352		G215	
	LYS		F353		I216	
	LYS		P354		F217	
	VAL		N355			
	SER		G356			
	SER		THR			
			PHE			

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 3.47Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.257 , 0.279 0.235 , 0.256	Depositor DCC
$R_{free}$ test set	816 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtrriage
Anisotropy	1.408	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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 [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	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:HG22	1:B:211:THR:O	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 [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	379/543 (70%)	329 (87%)	39 (10%)	11 (3%)	4	31
1	B	380/543 (70%)	326 (86%)	46 (12%)	8 (2%)	7	38
All	All	759/1086 (70%)	655 (86%)	85 (11%)	19 (2%)	5	34

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 [i](#)

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	13
1	B	315/459 (69%)	259 (82%)	56 (18%)	2	10
All	All	630/918 (69%)	522 (83%)	108 (17%)	2	12

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

Mol	Chain	Res	Type
1	B	49	ARG
1	B	159	LYS
1	B	334	ILE
1	B	61	MET
1	B	102	LYS

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

Mol	Chain	Res	Type
1	B	22	GLN
1	B	360	ASN
1	B	84	GLN
1	B	376	GLN
1	B	249	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 monosaccharides 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	B	1383	-	24,29,29	0.93	2 (8%)	29,45,45	1.88	6 (20%)
2	ADP	A	1383	-	24,29,29	0.96	1 (4%)	29,45,45	1.83	7 (24%)
3	PO4	A	1384	-	4,4,4	1.44	1 (25%)	6,6,6	1.60	1 (16%)
3	PO4	B	1384	-	4,4,4	1.32	1 (25%)	6,6,6	1.47	1 (16%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1384	PO4	P-O3	-2.63	1.46	1.54
3	B	1384	PO4	P-O3	-2.49	1.47	1.54
2	B	1383	ADP	C2'-C1'	2.34	1.57	1.53
2	B	1383	ADP	C5-C4	2.12	1.46	1.40
2	A	1383	ADP	C5-C4	2.01	1.46	1.40

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1383	ADP	PA-O3A-PB	-5.42	114.23	132.83
2	B	1383	ADP	PA-O3A-PB	-5.28	114.71	132.83
2	B	1383	ADP	N3-C2-N1	-4.15	122.19	128.68
2	A	1383	ADP	N3-C2-N1	-3.70	122.89	128.68
2	A	1383	ADP	C4-C5-N7	-2.79	106.50	109.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

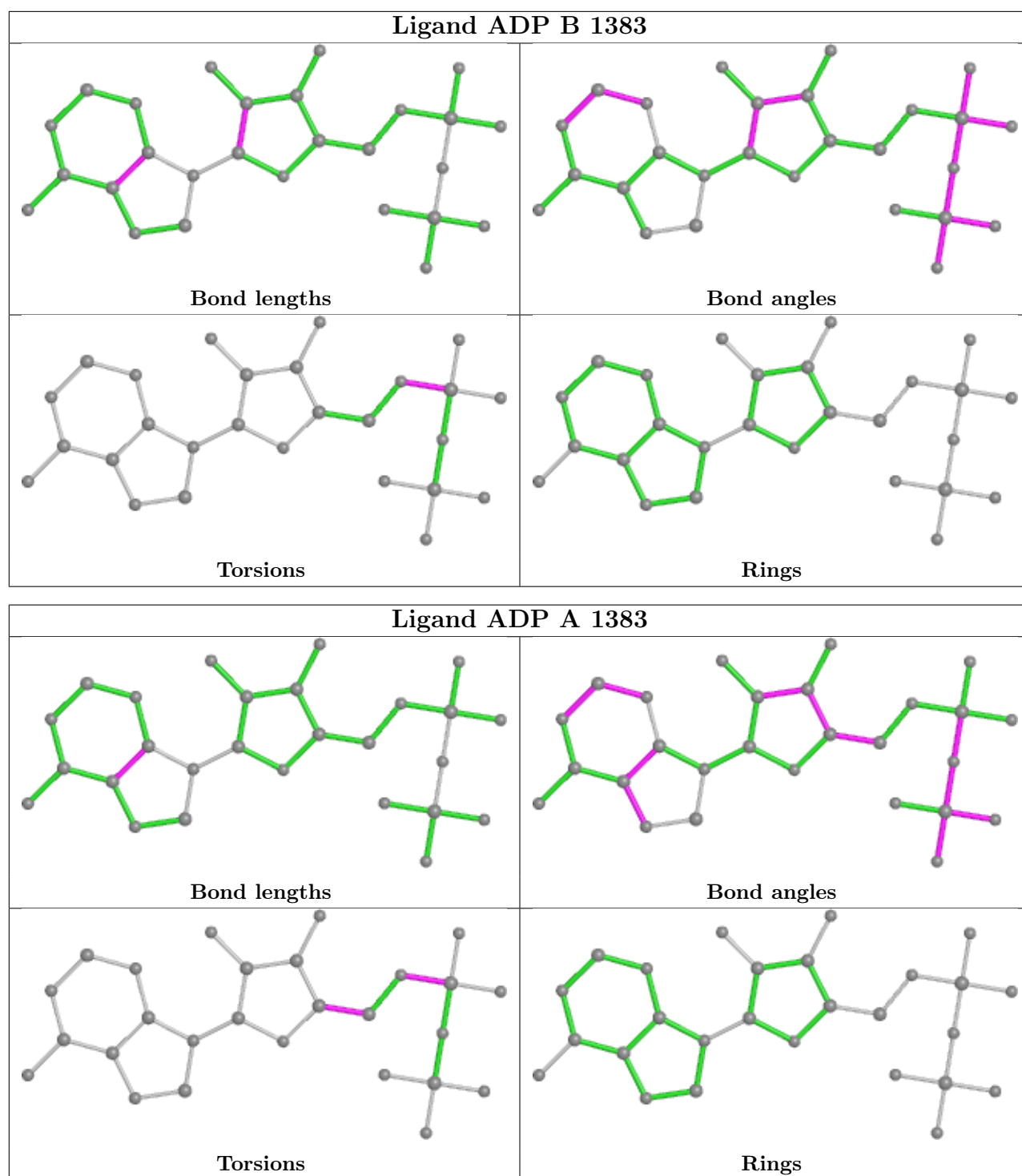
Mol	Chain	Res	Type	Atoms
2	B	1383	ADP	C5'-O5'-PA-O1A
2	A	1383	ADP	C3'-C4'-C5'-O5'
2	A	1383	ADP	O4'-C4'-C5'-O5'
2	B	1383	ADP	C5'-O5'-PA-O3A
2	A	1383	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1383	ADP	2	0
2	A	1383	ADP	1	0
3	B	1384	PO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	382:GLY	C	383:ASP	N	2.24

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	382/543 (70%)	-0.47	1 (0%) 94   91	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   95	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 monosaccharides in this entry.

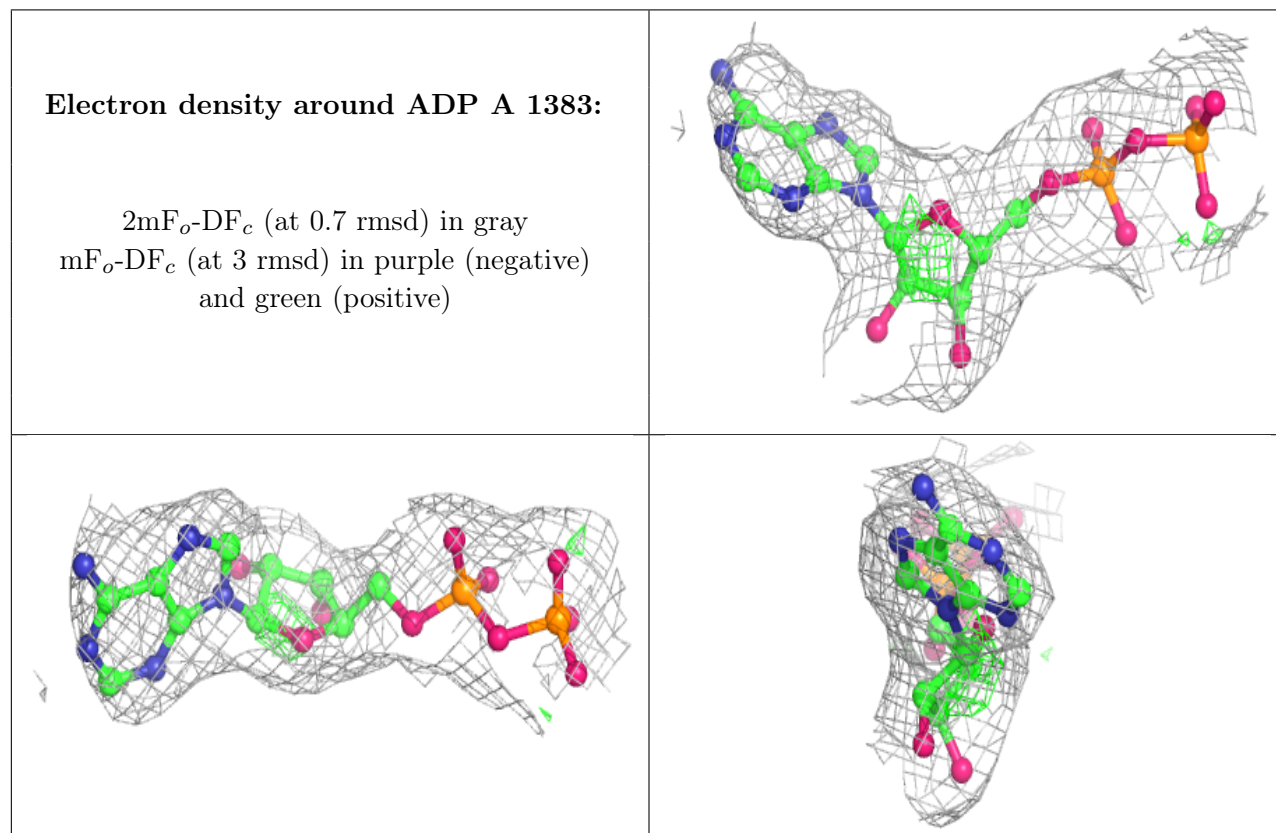
### 6.4 Ligands [i](#)

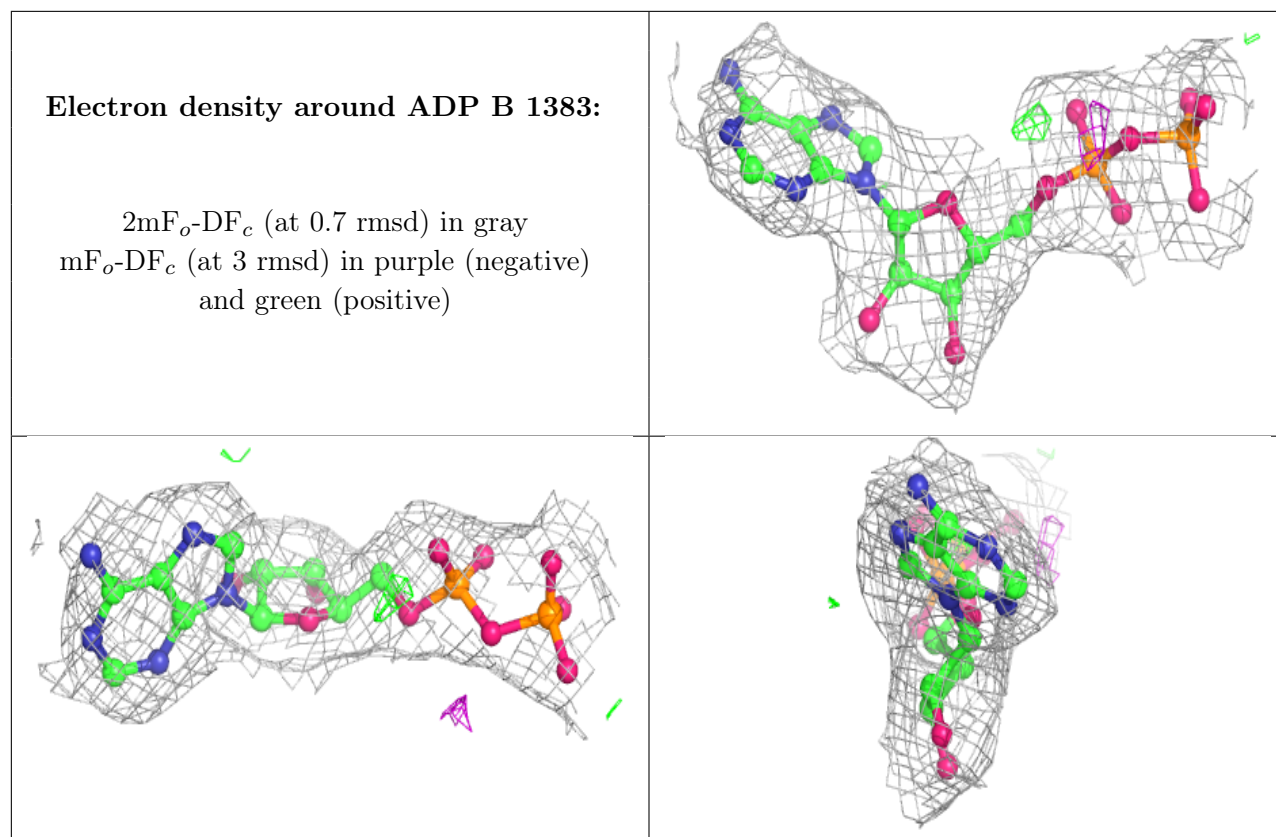
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ADP	A	1383	27/27	0.95	0.21	77,77,77,77	0
2	ADP	B	1383	27/27	0.96	0.18	61,61,61,61	0
3	PO4	A	1384	5/5	0.96	0.17	74,101,101,101	0
3	PO4	B	1384	5/5	0.98	0.11	37,37,37,165	0



The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.