



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1A6E  
Title : THERMOSOME-MG-ADP-ALF3 COMPLEX  
Authors : Ditzel, L.; Loewe, J.; Stock, D.; Stetter, K.-O.; Huber, H.; Huber, R.; Steinbacher, S.  
Deposited on : 1998-02-24  
Resolution : 3.20 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

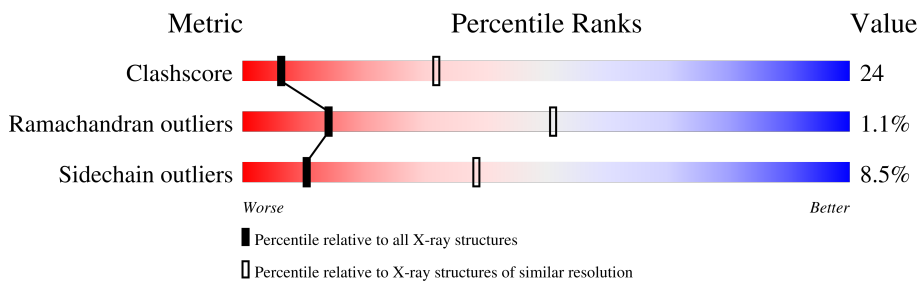
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	545	 49% 39% • 8%
2	B	543	 49% 39% • 8%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9390 atoms, of which 1742 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 THERMOSOME (ALPHA SUBUNIT).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	503	4668	2356	884	662	752	14	884	0	0

- Molecule 2 is a protein called THERMOSOME (BETA SUBUNIT).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	502	4656	2370	858	651	758	19	858	0	0

- 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		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



- Molecule 6 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
6	A	1	Total O 1 1	0	0
6	B	1	Total O 1 1	0	0



I511	A424	E346	L172
M512	Q425	R347	M272
I513	K426	V348	M273
L514	I427	E349	L274
R515	R430	Q350	E275
I516	Q431	R351	E276
V519	Q432	K352	M277
I520	L433	V353	V278
A521	E436	G354	I281
THR	LYS	E355	V284
SER	D440	D356	V287
SER	A441	Y357	I290
SER	I442	R358	T291
SER	E443	T359	Q292
SER	E444	F360	K293
SER	I445	V361	D296
ASN	P446	T362	D297
PRO	A450	G363	M298
PRO	L455	M366	A299
LYS	SER	P367	Q300
LYS	D456	K368	H301
GLY	P457	A369	I302
SER	I458	V370	L303
SER	D459	S371	Y304
GLU	I460	I372	S305
GLU	L461	L373	A310
SER	L462	V374	V311
SER	L462	G376	R312
GLU	M472	I389	R313
ASP	K473	T390	V314
	T474	D391	K223
	Y475	H394	V224
	G476	V395	M228
	I477	V396	V232
	I484	A399	A235
	M487	L400	K236
	V488	E401	I237
	K489	D402	A238
	M490	A405	L239
	G491	Y406	L240
	V492	A406	D241
	P495	A407	A242
	L496	G408	P243
	R497	G409	L244
	V498	T412	E245
	G499	E415	I246
	K500	I416	K247
	Q501	L420	K248
	A502	R421	P249
	I503	S422	E250
	T507	L423	R256
	A510	G343	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.80Å 167.80Å 202.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	92.5 (8.00-3.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.181 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP



## 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: ADP, MG, AF3

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	0.49	0/3812	0.74	2/5139 (0.0%)
2	B	0.52	0/3834	0.74	1/5166 (0.0%)
All	All	0.50	0/7646	0.74	3/10305 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	244	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	57	ASP	N-CA-C	5.18	125.00	111.00
1	A	160	SER	N-CA-C	5.15	124.91	111.00

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	A	3784	884	3935	191	0
2	B	3798	858	3892	195	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	7648	1742	7851	374	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 24.

The worst 5 of 374 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:218:ILE:HD11	1:A:321:LEU:HD11	1.22	1.11
2:B:172:LEU:HD22	2:B:389:ILE:HD11	1.46	0.96
1:A:281:LYS:HD2	1:A:305:GLU:HG3	1.48	0.95
2:B:50:LEU:HB2	2:B:58:VAL:HG13	1.48	0.93
2:B:64:VAL:HG22	2:B:95:THR:HG21	1.49	0.93

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	501/545 (92%)	450 (90%)	41 (8%)	10 (2%)	7	38
2	B	500/543 (92%)	463 (93%)	36 (7%)	1 (0%)	47	79
All	All	1001/1088 (92%)	913 (91%)	77 (8%)	11 (1%)	14	51

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	145	SER
1	A	377	THR
1	A	378	ASP
1	A	160	SER

### 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	411/442 (93%)	375 (91%)	36 (9%)	10	36
2	B	410/446 (92%)	376 (92%)	34 (8%)	11	40
All	All	821/888 (92%)	751 (92%)	70 (8%)	10	38

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	366	ASN
2	B	396	VAL
2	B	489	LYS
1	A	361	MET
1	A	354	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	480	ASN
2	B	87	GLN
2	B	394	HIS
2	B	35	ASN
2	B	108	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
5	AF3	A	899	6,3,4	0,3,3	-	-	-		
5	AF3	B	999	3,4,6	0,3,3	-	-	-		
4	ADP	A	898	3,5	24,29,29	1.29	4 (16%)	29,45,45	1.39	2 (6%)
4	ADP	B	998	3,5	24,29,29	1.18	4 (16%)	29,45,45	1.44	3 (10%)

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
4	ADP	A	898	3,5	-	4/12/32/32	0/3/3/3
4	ADP	B	998	3,5	-	1/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	898	ADP	C2'-C1'	-3.02	1.49	1.53
4	A	898	ADP	PB-O2B	2.71	1.65	1.54
4	B	998	ADP	PB-O2B	2.58	1.64	1.54
4	B	998	ADP	O4'-C1'	2.50	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	898	ADP	C5-N7	-2.36	1.31	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	998	ADP	N3-C2-N1	-5.93	119.41	128.68
4	A	898	ADP	N3-C2-N1	-5.69	119.79	128.68
4	A	898	ADP	C4-C5-N7	-2.62	106.67	109.40
4	B	998	ADP	C4-C5-N7	-2.48	106.82	109.40
4	B	998	ADP	O3B-PB-O3A	2.03	111.45	104.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

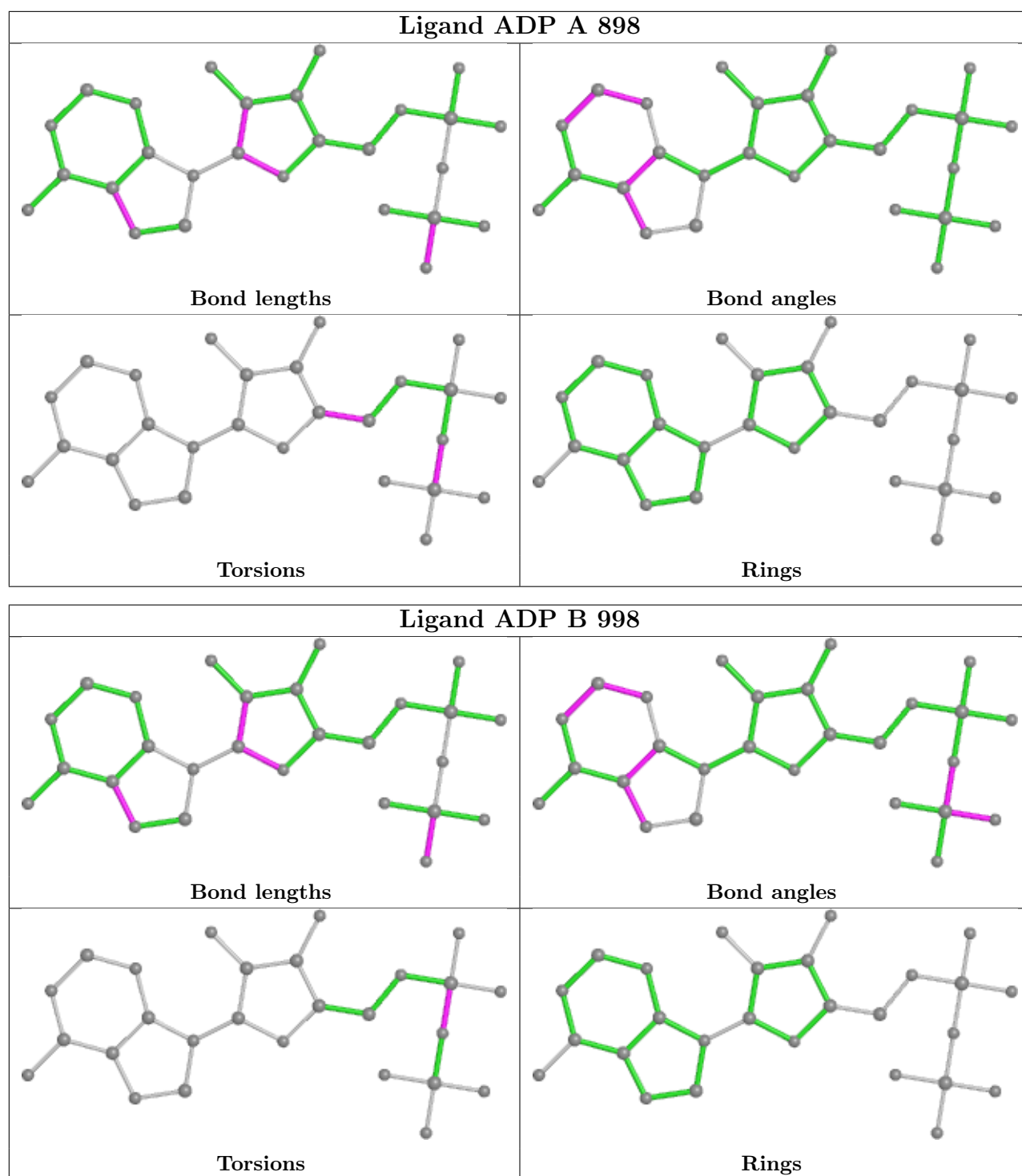
Mol	Chain	Res	Type	Atoms
4	A	898	ADP	PA-O3A-PB-O2B
4	A	898	ADP	C3'-C4'-C5'-O5'
4	A	898	ADP	PA-O3A-PB-O1B
4	A	898	ADP	PA-O3A-PB-O3B
4	B	998	ADP	PB-O3A-PA-O1A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	898	ADP	1	0
4	B	998	ADP	3	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

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.