



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 20, 2018 – 06:41 pm GMT

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)

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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

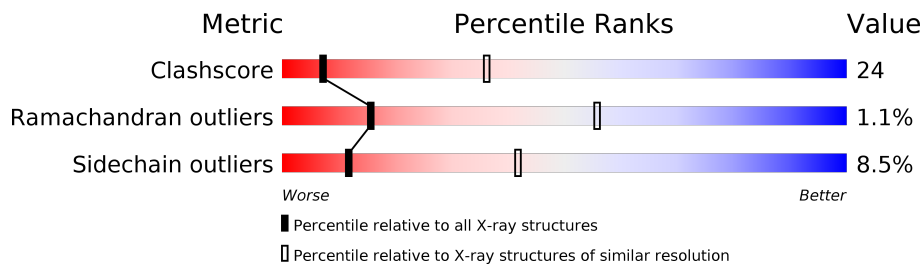
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	122078	1092 (3.20-3.20)
Ramachandran outliers	120005	1075 (3.20-3.20)
Sidechain outliers	119972	1074 (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 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	A	545	
2	B	543	

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
1	A	503	Total	C	H	N	O	S	884	0	0
			4668	2356	884	662	752	14			

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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

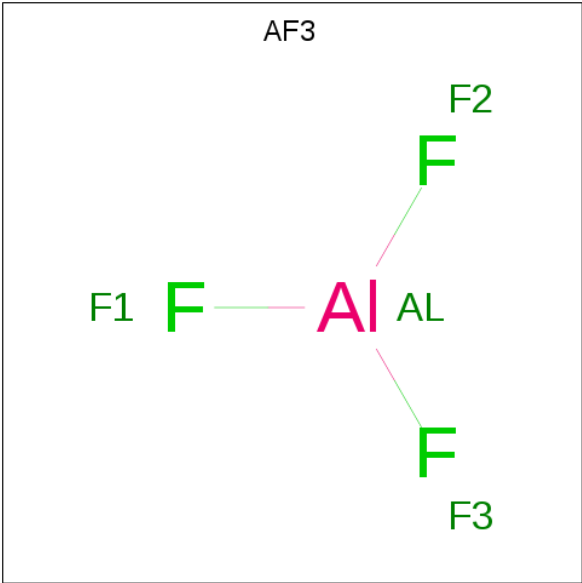
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			4	1	3		
5	B	1	Total	Al	F	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	O 1	0	0
6	B	1	Total 1	O 1	0	0

I511	E346	A424	N272	N366	N472	I484	N487	P495	V519	N273	N367	N473	V488	I496	V520	D296	K310	L322	A325	G327	A328	S329	I330	V331	S332	I333	I334	I337	S338	S339	S340	D341	L342	G343
M512	R347	Q425	M272	N368	K472	I487	V489	R496	I513	R348	K368	K473	K488	I497	A501	D297	V311	L323	A326	G328	A329	I331	V332	S333	I334	I337	S338	S339	S340	D341	L342	G343		
I513	V348	K426	L274	V350	R430	N488	K489	I497	I514	E349	A369	T474	N490	R497	A502	A298	R312	L324	A327	G329	S330	I332	V333	S334	I337	S338	S339	S340	D341	L342	G343			
R515	E350	I427	I275	W277	Q431	G476	N491	V498	I516	R276	V370	Y475	G491	V499	A503	Q300	R313	L325	A328	G330	S331	I333	V334	S335	I337	S338	S339	S340	D341	L342	G343			
I516	W277	I428	I276	W278	Q432	I477	N492	V499	I517	E351	S371	I478	G492	G499	A504	H301	R314	L326	A329	G331	S332	I334	V335	S336	I337	S338	S339	S340	D341	L342	G343			
V519	K352	Q433	L433	E436	Q434	L462	N493	V500	I520	V353	L372	L461	G493	G500	A505	I302	R315	L327	A330	G332	S333	I335	V336	S337	I337	S338	S339	S340	D341	L342	G343			
I520	G354	L434	E437	D440	Q435	L463	N494	V501	A521	G355	L373	L464	G494	G501	A506	H303	R316	L328	A331	G333	S334	I336	V337	S338	I337	S338	S339	S340	D341	L342	G343			
A521	D356	L435	E438	A441	Q436	L464	N495	V502	I521	E356	L374	L465	G495	G502	A507	H304	R317	L329	A332	G334	S335	I337	V338	S339	I337	S338	S339	S340	D341	L342	G343			
THR	D357	L436	E439	A442	Q437	L465	N496	V503	I522	E357	L375	L466	G496	G503	A508	H305	R318	L330	A333	G335	S336	I338	V339	S340	I337	S338	S339	S340	D341	L342	G343			
LYS	D358	L437	E440	A443	Q438	L466	N497	V504	I523	E358	L376	L467	G497	G504	A509	H306	R319	L331	A334	G336	S337	I339	V340	S341	I337	S338	S339	S340	D341	L342	G343			
SER	D359	L438	E441	A444	Q439	L467	N498	V505	I524	E359	L377	L468	G498	G505	A510	H307	R320	L332	A335	G337	S338	I340	V341	S342	I337	S338	S339	S340	D341	L342	G343			
SER	D360	L439	E442	A445	Q440	L468	N499	V506	I525	E360	L378	L469	G499	G506	A511	H308	R321	L333	A336	G338	S339	I341	V342	S343	I337	S338	S339	S340	D341	L342	G343			
SER	D361	L440	E443	A446	Q441	L469	N500	V507	I526	E361	L379	L470	G500	G507	A512	H309	R322	L334	A337	G339	S340	I342	V343	S344	I337	S338	S339	S340	D341	L342	G343			
SER	D362	L441	E444	A447	Q442	L470	N501	V508	I527	E362	L380	L471	G501	G508	A513	H310	R323	L335	A338	G340	S341	I343	V344	S345	I337	S338	S339	S340	D341	L342	G343			
SER	D363	L442	E445	A448	Q443	L471	N502	V509	I528	E363	L381	L472	G502	G509	A514	H311	R324	L336	A339	G341	S342	I344	V345	S346	I337	S338	S339	S340	D341	L342	G343			
ASN	D364	L443	E446	A449	Q444	L472	N503	V510	I529	E364	L382	L473	G503	G510	A515	H312	R325	L337	A340	G342	S343	I345	V346	S347	I337	S338	S339	S340	D341	L342	G343			
PRO	D365	L444	E447	A450	Q445	L473	N504	V511	I530	E365	L383	L474	G504	G511	A516	H313	R326	L338	A341	G343	S344	I346	V347	S348	I337	S338	S339	S340	D341	L342	G343			
GLY	D366	L445	E448	A451	Q446	L474	N505	V512	I531	E366	L384	L475	G505	G512	A517	H314	R327	L339	A342	G344	S345	I347	V348	S349	I337	S338	S339	S340	D341	L342	G343			
SER	D367	L446	E449	A452	Q447	L475	N506	V513	I532	E367	L385	L476	G506	G513	A518	H315	R328	L340	A343	G345	S346	I348	V349	S350	I337	S338	S339	S340	D341	L342	G343			
SER	D368	L447	E450	A453	Q448	L476	N507	V514	I533	E368	L386	L477	G507	G514	A519	H316	R329	L341	A344	G346	S347	I349	V350	S351	I337	S338	S339	S340	D341	L342	G343			
SER	D369	L448	E451	A454	Q449	L477	N508	V515	I534	E369	L387	L478	G508	G515	A520	H317	R330	L342	A345	G347	S348	I350	V351	S352	I337	S338	S339	S340	D341	L342	G343			
SER	D370	L449	E452	A455	Q450	L478	N509	V516	I535	E370	L388	L479	G509	G516	A521	H318	R331	L343	A346	G348	S349	I351	V352	S353	I337	S338	S339	S340	D341	L342	G343			
SER	D371	L450	E453	A456	Q451	L479	N510	V517	I536	E371	L389	L480	G510	G517	A522	H319	R332	L344	A347	G349	S350	I352	V353	S354	I337	S338	S339	S340	D341	L342	G343			
SER	D372	L451	E454	A457	Q452	L480	N511	V518	I537	E372	L390	L481	G511	G518	A523	H320	R333	L345	A348	G350	S351	I353	V354	S355	I337	S338	S339	S340	D341	L342	G343			
SER	D373	L452	E455	A458	Q453	L481	N512	V519	I538	E373	L391	L482	G512	G519	A524	H321	R334	L346	A349	G351	S352	I354	V355	S356	I337	S338	S339	S340	D341	L342	G343			
SER	D374	L453	E456	A459	Q454	L482	N513	V520	I539	E374	L392	L483	G513	G520	A525	H322	R335	L347	A350	G352	S353	I355	V356	S357	I337	S338	S339	S340	D341	L342	G343			
SER	D375	L454	E457	A460	Q455	L483	N514	V521	I540	E375	L393	L484	G514	G521	A526	H323	R336	L348	A351	G353	S354	I356	V357	S358	I337	S338	S339	S340	D341	L342	G343			
SER	D376	L455	E458	A461	Q456	L484	N515	V522	I541	E376	L394	L485	G515	G522	A527	H324	R337	L349	A352	G354	S355	I357	V358	S359	I337	S338	S339	S340	D341	L342	G343			
SER	D377	L456	E459	A462	Q457	L485	N516	V523	I542	E377	L395	L486	G516	G523	A528	H325	R338	L350	A353	G355	S356	I358	V359	S360	I337	S338	S339	S340	D341	L342	G343			
SER	D378	L457	E460	A463	Q458	L486	N517	V524	I543	E378	L396	L487	G517	G524	A529	H326	R339	L351	A354	G356	S357	I359	V360	S361	I337	S338	S339	S340	D341	L342	G343			
SER	D379	L458	E461	A464	Q459	L487	N518	V525	I544	E379	L397	L488	G518	G525	A530	H327	R340	L352	A355	G357	S358	I360	V361	S362	I337	S338	S339	S340	D341	L342	G343			
SER	D380	L459	E462	A465	Q460	L488	N519	V526	I545	E380	L398	L489	G519	G526	A531	H328	R341	L353	A356	G358	S359	I361	V362	S363	I337	S338	S339	S340	D341	L342	G343			
SER	D381	L460	E463	A466	Q461	L489	N520	V527	I546	E381	L399	L490	G520	G527	A532	H329	R342	L354	A357	G359	S360	I362	V363	S364	I337	S338	S339	S340	D341	L342	G343			
SER	D382	L461	E464	A467	Q462	L490	N521	V528	I547	E382	L400	L491	G521	G528	A533	H330	R343	L355	A358	G360	S361	I363	V364	S365	I337	S338	S339	S340	D341	L342	G343			
SER	D383	L462	E465	A468	Q463	L491	N522	V529	I548	E383	L401	L492	G522	G529	A534	H331	R344	L356	A359	G361	S362	I364	V365	S366	I337	S338	S339	S340	D341	L342	G343			
SER	D384	L463	E466	A469	Q464	L492	N523	V530	I549	E384	L402	L493	G523	G530	A535	H332	R345	L357	A360	G362	S363	I365	V366	S367	I337	S338	S339	S340	D341	L342	G343			
SER	D385	L464	E467	A470	Q465	L493	N524	V531	I550	E385	L403	L494	G524	G531	A536	H333	R346	L358	A361	G363	S364	I366	V367	S368	I337	S338	S339	S340	D341	L342	G343			
SER	D386	L465	E468	A471	Q466	L494	N525	V532	I551	E386	L404	L495	G525	G532	A537	H334	R347	L359	A362	G364	S365	I367	V368	S369	I337	S338	S339	S340	D341	L342	G343			
SER	D387	L466	E469	A472	Q467	L495	N526	V533	I552	E387	L405	L496	G526	G533	A538	H335	R348	L360	A363	G365	S366	I368	V369	S370	I337	S338	S339	S340	D341	L342	G343			
SER	D388	L467	E470	A473	Q468	L496	N527	V534	I553	E388	L406	L497	G527	G534	A539	H336	R349	L361	A364	G366	S367	I369	V370	S371	I337	S338	S339	S340	D341	L342	G343			
SER	D389	L468	E471	A474	Q469	L497	N528	V535	I554	E389	L407	L498	G528	G535	A540	H337	R350	L362	A365	G367	S368	I370	V371	S372	I337	S338	S339	S340	D341	L342	G343			
SER	D390	L469	E472	A475	Q470	L498	N529	V536	I555	E390	L408	L499	G529	G536	A541	H338	R351	L363	A366	G368	S369	I371	V372	S373	I337	S338	S339	S340	D341	L342	G343			
SER	D391	L470	E473	A476	Q471	L499	N530	V537	I556	E391	L409	L500	G530	G537	A542	H339	R352	L364	A367	G369	S370	I372	V373	S374	I337	S338	S339	S340	D341	L342	G343			
SER	D392	L471	E474	A477	Q472	L500	N531	V538	I557	E392	L410	L501	G531	G538	A543	H340	R353	L365	A368	G370	S371	I373	V374	S375	I337	S338	S339	S340	D341	L342	G343			
SER	D393	L472	E475	A478	Q473	L501	N532	V539	I558	E393	L411	L502	G532	G539	A544	H341	R354	L366	A369	G371	S372	I374	V375	S376	I337	S338	S339	S340	D341	L342	G343			
SER	D394	L473	E476	A479	Q474	L502	N533	V540	I559	E394	L412	L503	G533	G540	A545	H342	R355	L367	A370	G372	S373	I375	V376	S377	I337	S338	S339	S340	D341	L342	G343			
SER	D395	L474	E477	A480	Q475	L503	N534	V541	I560	E395	L413	L504	G534	G541	A546	H343	R356	L368	A371	G373	S374	I376	V377	S378	I337	S338	S339	S340	D341	L342	G343			
SER	D396	L475	E478	A481	Q476	L504	N535	V542																										

4 Data and refinement statistics

Xtriage (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, α , β , γ	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.	Xtriage
Total number of atoms	9390	wwPDB-VP
Average B, all atoms (Å ²)	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: MG, ADP, 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

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	501/545 (92%)	450 (90%)	41 (8%)	10 (2%)	8	42
2	B	500/543 (92%)	463 (93%)	36 (7%)	1 (0%)	49	83
All	All	1001/1088 (92%)	913 (91%)	77 (8%)	11 (1%)	16	56

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%)	11	39
2	B	410/446 (92%)	376 (92%)	34 (8%)	12	43
All	All	821/888 (92%)	751 (92%)	70 (8%)	12	42

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

Mol	Chain	Res	Type
1	A	467	ASP
2	B	67	LEU
2	B	462	LEU
1	A	478	LEU
1	A	516	ASP

Some 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	424	ASN
1	A	480	ASN
2	B	394	HIS
1	A	431	GLN
1	A	451	ASN

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 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$
4	ADP	A	898	3,5	25,29,29	1.24	4 (16%)	25,45,45	2.33	3 (12%)
5	AF3	A	899	3,4,6	0,3,3	0.00	-	0,3,3	0.00	-
4	ADP	B	998	3,5	25,29,29	1.24	4 (16%)	25,45,45	2.38	2 (8%)
5	AF3	B	999	3,4,6	0,3,3	0.00	-	0,3,3	0.00	-

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	-	0/12/32/32	0/3/3/3
5	AF3	A	899	3,4,6	-	0/0/0/0	0/0/0/0
4	ADP	B	998	3,5	-	0/12/32/32	0/3/3/3
5	AF3	B	999	3,4,6	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	998	ADP	C8-N9	-3.13	1.33	1.36
4	A	898	ADP	C8-N9	-2.80	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	898	ADP	C5-N7	-2.43	1.31	1.39
4	B	998	ADP	C5-N7	-2.22	1.31	1.39
4	A	898	ADP	O4'-C1'	2.17	1.44	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	998	ADP	N3-C2-N1	-11.04	119.41	128.86
4	A	898	ADP	N3-C2-N1	-10.61	119.79	128.86
4	A	898	ADP	C4-C5-N7	-2.84	106.67	109.41
4	B	998	ADP	C4-C5-N7	-2.68	106.82	109.41
4	A	898	ADP	C4'-O4'-C1'	-2.08	107.66	109.83

There are no chirality outliers.

There are no torsion outliers.

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

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.