



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:51 AM UTC

PDB ID : 1A6E / pdb_00001a6e
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

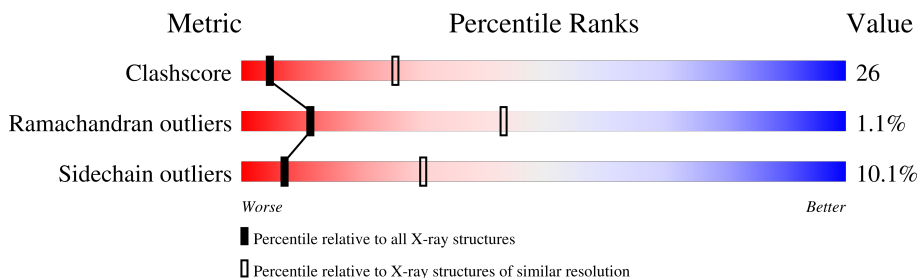
1 Overall quality at a glance

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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (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 ≥ 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	
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			

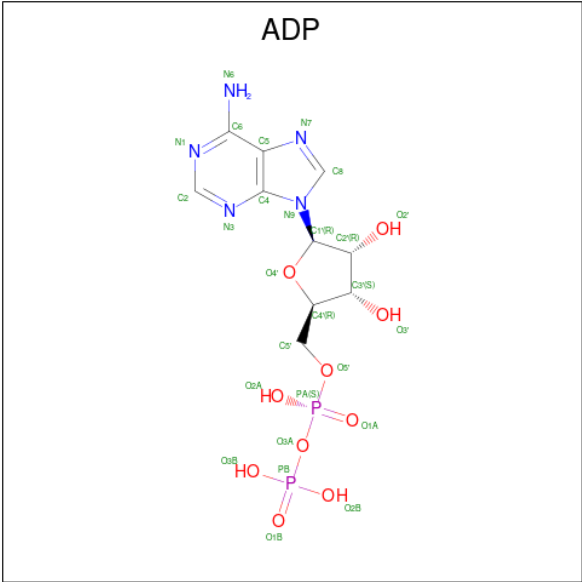
- Molecule 2 is a protein called THERMOSOME (BETA SUBUNIT).

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 (CCD ID: MG) (formula: Mg).

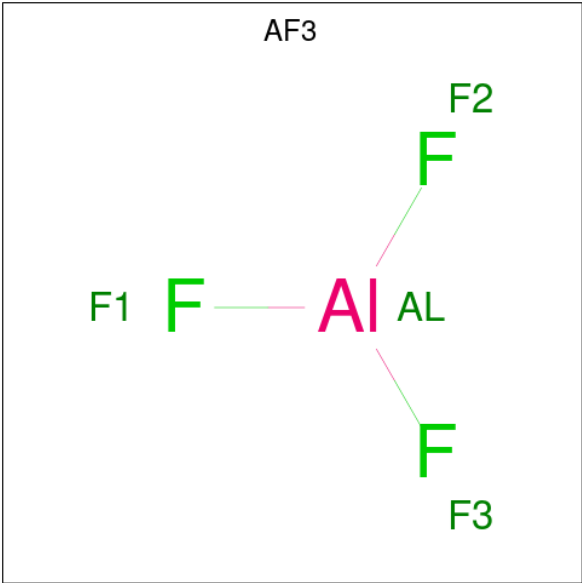
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



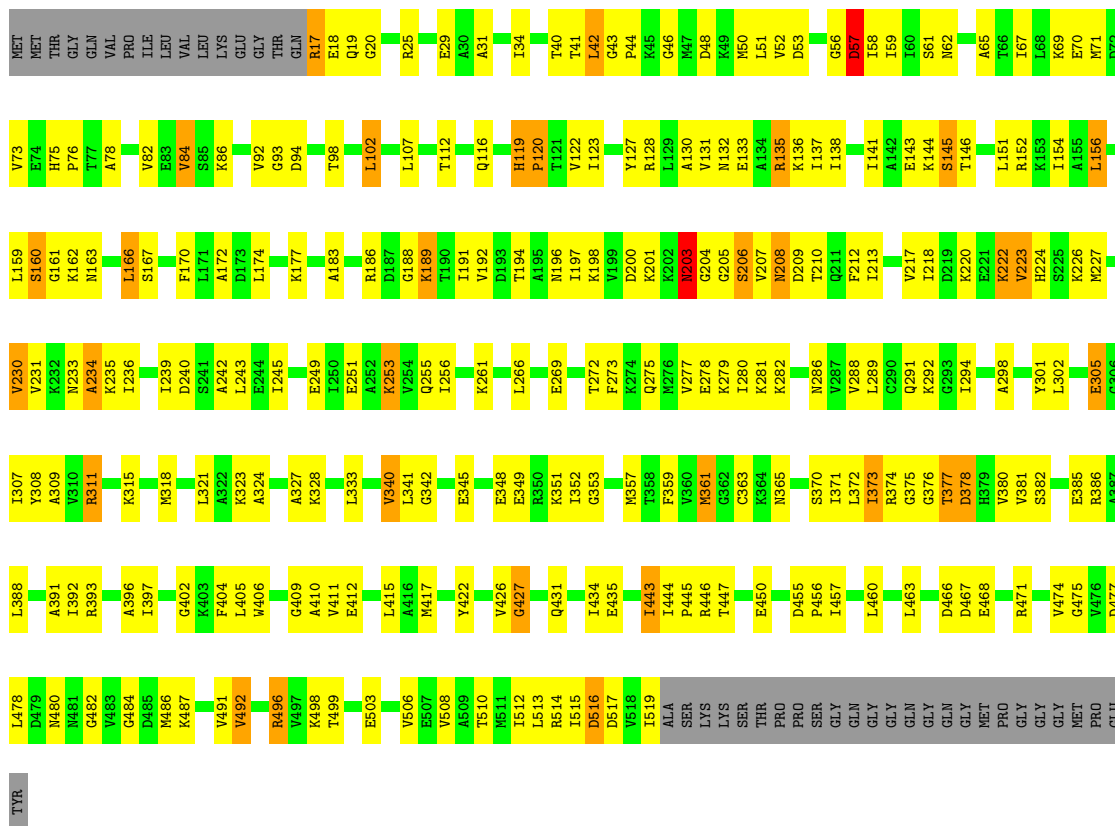
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			4	1	3		
5	B	1	Total	Al	F	0	0
			4	1	3		

- Molecule 6 is water.

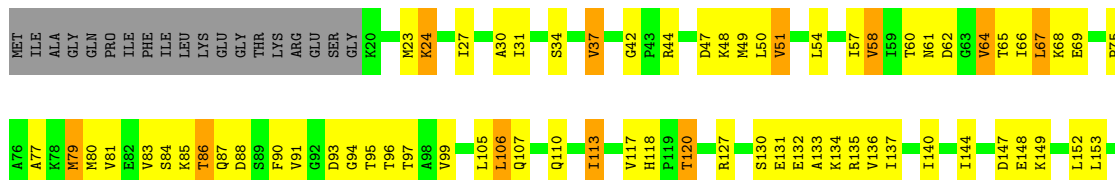
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	1	Total	O	0	0
			1	1		

Note EDS was not executed.

Chain A: 47% 40% 6% 8%



Chain B: 45% 39% 7% 8%



M487	V488	K489	N490	G491	V492	P495	I496	R497	V498	G499	K500	Q501	A502	T503	T507	A510	I511	M512	I513	L514	R515	I516	V519	I520	A521	THR	LYS	SER	SER	SER	SER	SER	ASN	PRO	PRO	LYS	LYS	SER	GLY	SER	SER	SER	SER	GLU	SER	GLU	ASP							
D402	Y405	A406	A407	G408	G409	T412	E415	I416	L420	R421	S422	Y423	A424	Q425	K426	I427	R430	Q431	Q432	L433	E436	D440	A441	I442	E443	E444	I445	P446	A450	L455	D456	P457	I458	D459	I460	L461	L462	A469	K470	G471	N472	K473	T474	Y475	G476	I477	I484							
G327	A328	S329	I330	V331	S332	T333	I334	I337	S338	S339	S340	D341	L342	G343	T344	A345	E346	R347	V348	E349	Q350	V351	K352	V353	G354	E355	D356	Y357	M358	T359	F360	V361	T362	G363	N366	F367	K368	A369	V370	S371	I372	L373	V374	R375	G376	I389	T390	D391	H394	V395	V396	A399	L400	E401
T158	N161	S162	K163	S164	A165	L172	Y177	E178	E185	G189	Y192	F195	D196	N197	I198	Q199	V200	V201	K202	K203	Q204	A207	I208	D209	D210	T211	Q212	I213	I214	N215	G216	I217	I218	V219	D220	K221	E222	K223	V224	M228	V232	A235	K236	I237	A238	L239	L240	D241						
A242	P243	L244	E245	K247	K248	P249	E250	L255	R256	Q269	N272	M273	L274	R275	E276	M277	V278	I281	V284	N287	I290	T291	Q292	K293	D296	D297	M298	A299	Q300	H301	Y302	L303	L304	S304	R305	A310	V311	R312	R313	V314	K315	K316	S317	D318	M319	L322	A325	T326						

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: AF3, 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	A	0.65	0/3812	1.10	24/5139 (0.5%)
2	B	0.69	1/3834 (0.0%)	1.09	19/5166 (0.4%)
All	All	0.67	1/7646 (0.0%)	1.10	43/10305 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	ILE	CA-CB	6.05	1.62	1.54

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	430	ARG	N-CA-C	-7.43	102.87	112.23
2	B	42	GLY	CA-C-N	7.24	126.87	119.56
2	B	42	GLY	C-N-CA	7.24	126.87	119.56
2	B	64	VAL	CB-CA-C	-7.24	102.37	112.14
1	A	43	GLY	CA-C-N	7.22	128.86	119.84

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	200	0
2	B	3798	858	3892	211	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
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	399	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 26.

The worst 5 of 399 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%)	6 31
2	B	500/543 (92%)	463 (93%)	36 (7%)	1 (0%)	43 73
All	All	1001/1088 (92%)	913 (91%)	77 (8%)	11 (1%)	11 43

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 ⓘ

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%)	376 (92%)	35 (8%)	10	37
2	B	410/446 (92%)	362 (88%)	48 (12%)	5	23
All	All	821/888 (92%)	738 (90%)	83 (10%)	7	30

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	248	LYS
2	B	412	THR
2	B	255	LEU
2	B	344	THR
2	B	489	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	ASN
2	B	394	HIS
1	A	480	ASN
2	B	490	ASN
2	B	300	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	5,3	28,29,29	1.43	4 (14%)	43,45,45	2.07	9 (20%)
5	AF3	B	999	3,6,4	0,3,3	-	-	-		
5	AF3	A	899	3,6,4	0,3,3	-	-	-		
4	ADP	B	998	5,3	28,29,29	1.33	4 (14%)	43,45,45	2.05	9 (20%)

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	5,3	-	6/16/32/32	0/3/3/3
4	ADP	B	998	5,3	-	2/16/32/32	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	C5-N7	-4.35	1.31	1.39
4	B	998	ADP	C5-N7	-3.95	1.31	1.39
4	A	898	ADP	C4-N9	-2.89	1.31	1.37
4	B	998	ADP	C4-N9	-2.84	1.31	1.37
4	A	898	ADP	PB-O2B	2.82	1.65	1.54

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	998	ADP	N3-C2-N1	-6.06	119.41	128.58
4	A	898	ADP	N3-C2-N1	-5.81	119.79	128.58
4	A	898	ADP	C5-C4-N3	-5.51	119.13	126.72
4	B	998	ADP	C5-C4-N3	-5.49	119.16	126.72
4	B	998	ADP	C2-N3-C4	4.49	122.80	111.83

There are no chirality outliers.

5 of 8 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

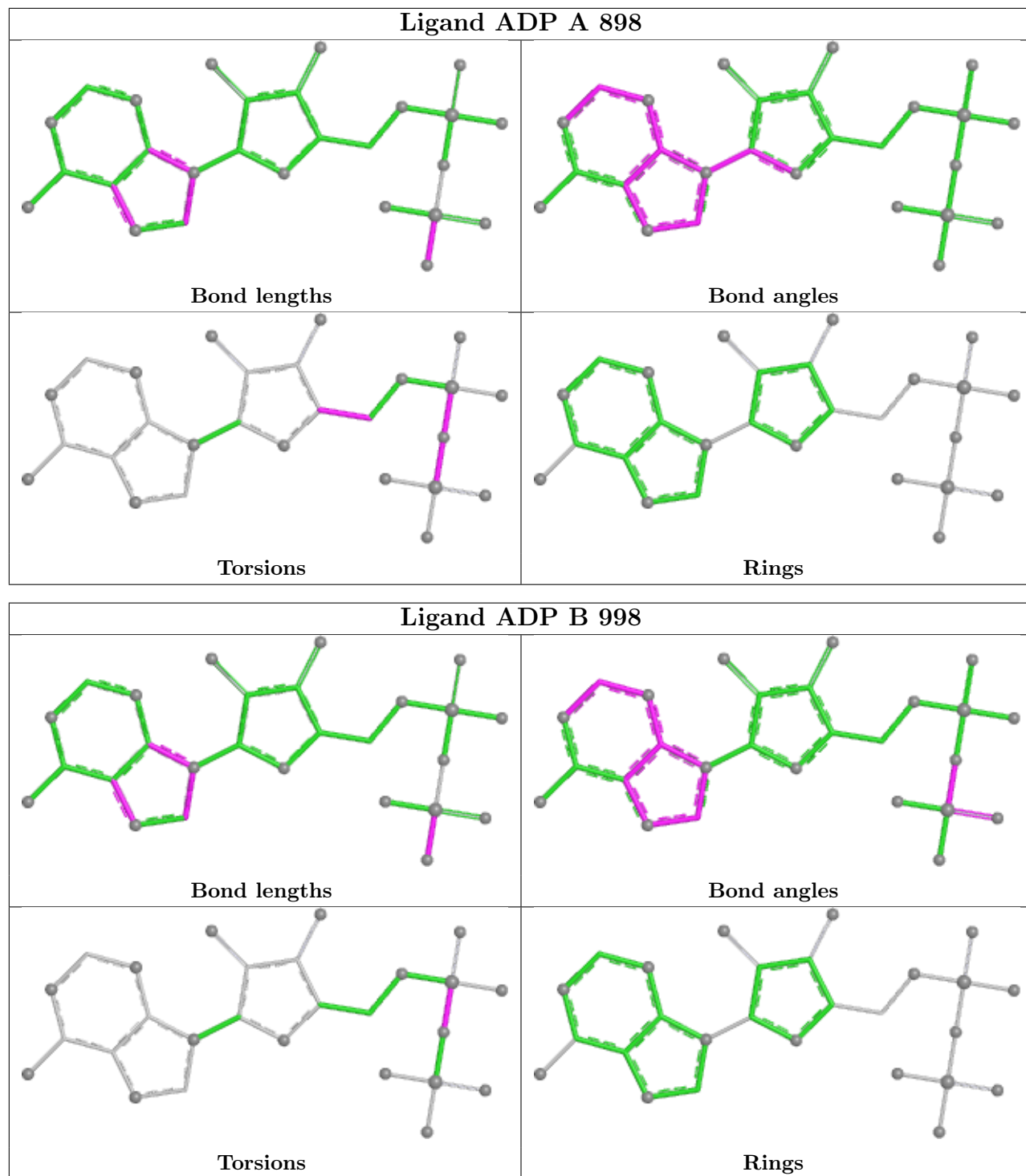
There are no ring outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.