



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:00 PM UTC

PDB ID : 1F9A / pdb_00001f9a
Title : CRYSTAL STRUCTURE ANALYSIS OF NMN ADENYLYLTRANSFERASE FROM METHANOCOCCUS JANNASCHII
Authors : D'Angelo, I.; Raffaelli, N.; Dabusti, V.; Lorenzi, T.; Magni, G.; Rizzi, M.
Deposited on : 2000-07-09
Resolution : 2.00 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

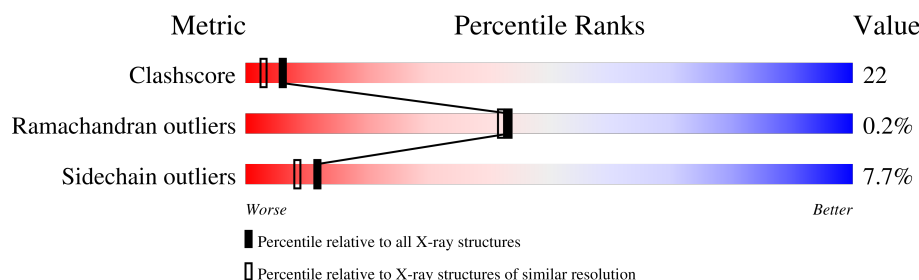
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	168	54% 35% 7% . .
1	B	168	46% 38% 11% . .
1	C	168	54% 35% 8% . .
1	D	168	40% 37% 16% 5% .
1	E	168	47% 41% 6% . .
1	F	168	58% 32% 6% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ATP	E	704	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8923 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 HYPOTHETICAL PROTEIN MJ0541.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1341	869	231	238	3			
1	B	164	Total	C	N	O	S	0	0	0
			1341	869	231	238	3			
1	C	164	Total	C	N	O	S	0	0	0
			1338	866	231	238	3			
1	D	164	Total	C	N	O	S	0	0	0
			1348	875	231	239	3			
1	E	164	Total	C	N	O	S	0	0	0
			1348	875	231	239	3			
1	F	164	Total	C	N	O	S	0	0	0
			1351	876	231	241	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	MET	conflict	UNP Q57961
B	1	LEU	MET	conflict	UNP Q57961
C	1	LEU	MET	conflict	UNP Q57961
D	1	LEU	MET	conflict	UNP Q57961
E	1	LEU	MET	conflict	UNP Q57961
F	1	LEU	MET	conflict	UNP Q57961

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

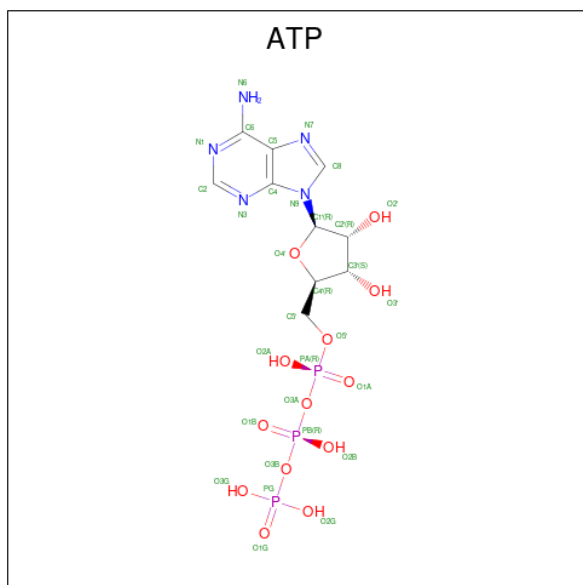
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is water.

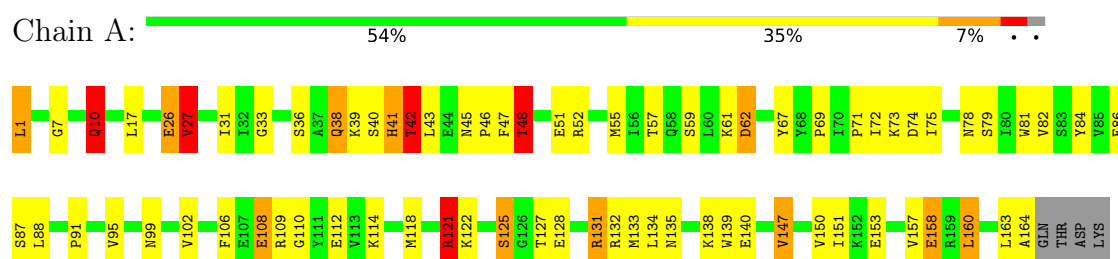
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total 105	O 105	0	0
4	B	100	Total 100	O 100	0	0
4	C	103	Total 103	O 103	0	0
4	D	93	Total 93	O 93	0	0
4	E	122	Total 122	O 122	0	0
4	F	141	Total 141	O 141	0	0

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: HYPOTHETICAL PROTEIN MJ0541



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.77Å 112.64Å 79.87Å 90.00° 116.94° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	96.0 (20.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8923	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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, ATP

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	0.99	1/1371 (0.1%)	2.14	60/1849 (3.2%)
1	B	0.94	0/1371	2.19	69/1849 (3.7%)
1	C	0.99	0/1368	2.01	45/1845 (2.4%)
1	D	1.00	1/1379 (0.1%)	2.22	77/1860 (4.1%)
1	E	1.02	2/1379 (0.1%)	2.07	54/1860 (2.9%)
1	F	1.07	2/1382 (0.1%)	1.94	35/1864 (1.9%)
All	All	1.00	6/8250 (0.1%)	2.10	340/11127 (3.1%)

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	0	5
1	B	1	4
1	C	1	3
1	D	0	14
1	E	1	9
1	F	1	2
All	All	4	37

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	70	ILE	N-CA	6.10	1.50	1.45
1	E	87	SER	CA-CB	5.63	1.62	1.53
1	E	72	ILE	C-O	5.62	1.30	1.24
1	F	85	VAL	N-CA	5.49	1.52	1.46
1	A	87	SER	CA-CB	5.42	1.61	1.53

The worst 5 of 340 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ARG	NE-CZ-NH2	19.42	136.68	119.20
1	E	75	ILE	O-C-N	-12.38	109.97	122.97
1	F	75	ILE	O-C-N	-12.35	109.75	122.97
1	A	48	THR	N-CA-CB	-12.31	93.52	110.38
1	D	68	TYR	O-C-N	11.97	128.45	121.27

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	48	THR	CB
1	C	48	THR	CB
1	E	48	THR	CB
1	F	48	THR	CB

5 of 37 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	GLY	Mainchain
1	A	125	SER	Mainchain
1	A	7	GLY	Mainchain
1	A	81	TRP	Mainchain
1	A	95	VAL	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	1341	0	1375	53	0
1	B	1341	0	1375	67	0
1	C	1338	0	1366	60	0
1	D	1348	0	1382	77	0
1	E	1348	0	1382	60	0
1	F	1351	0	1384	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	31	0	11	1	0
3	B	31	0	12	0	0
3	C	31	0	12	1	0
3	D	31	0	12	6	0
3	E	31	0	11	0	0
3	F	31	0	12	0	0
4	A	105	0	0	16	0
4	B	100	0	0	16	0
4	C	103	0	0	9	0
4	D	93	0	0	13	0
4	E	122	0	0	17	0
4	F	141	0	0	19	0
All	All	8923	0	8334	373	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 22.

The worst 5 of 373 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:E:118:MET:HE3	1:E:121:ARG:HD2	1.16	1.16
1:A:55:MET:SD	4:A:791:HOH:O	2.07	1.13
1:A:118:MET:HE3	1:A:121:ARG:HD2	1.19	1.11
1:C:118:MET:HE3	1:C:121:ARG:HD2	1.27	1.11
1:B:134:LEU:HD21	1:B:161:ARG:HA	1.18	1.10

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	162/168 (96%)	157 (97%)	5 (3%)	0	100	100
1	B	162/168 (96%)	154 (95%)	7 (4%)	1 (1%)	21	17
1	C	162/168 (96%)	155 (96%)	7 (4%)	0	100	100
1	D	162/168 (96%)	152 (94%)	10 (6%)	0	100	100
1	E	162/168 (96%)	153 (94%)	8 (5%)	1 (1%)	21	17
1	F	162/168 (96%)	155 (96%)	7 (4%)	0	100	100
All	All	972/1008 (96%)	926 (95%)	44 (4%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	35	GLY
1	B	148	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	146/152 (96%)	134 (92%)	12 (8%)	10	7
1	B	146/152 (96%)	134 (92%)	12 (8%)	10	7
1	C	145/152 (95%)	136 (94%)	9 (6%)	16	13
1	D	147/152 (97%)	134 (91%)	13 (9%)	9	6
1	E	147/152 (97%)	134 (91%)	13 (9%)	9	6
1	F	148/152 (97%)	139 (94%)	9 (6%)	17	14
All	All	879/912 (96%)	811 (92%)	68 (8%)	12	8

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	125	SER
1	F	17	LEU
1	F	121	ARG

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Mol	Chain	Res	Type
1	C	1	LEU
1	B	144	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	78	ASN
1	E	38	GLN
1	F	41	HIS
1	D	141	HIS
1	E	41	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
3	ATP	F	705	2	32,33,33	1.52	4 (12%)	48,52,52	1.48	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	B	701	-	32,33,33	1.36	4 (12%)	48,52,52	1.45	6 (12%)
3	ATP	D	703	2	32,33,33	1.31	2 (6%)	48,52,52	1.84	9 (18%)
3	ATP	E	704	2	32,33,33	1.55	5 (15%)	48,52,52	2.56	18 (37%)
3	ATP	A	700	2	32,33,33	1.45	5 (15%)	48,52,52	1.81	11 (22%)
3	ATP	C	702	2	32,33,33	1.38	3 (9%)	48,52,52	1.36	7 (14%)

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
3	ATP	F	705	2	-	2/22/38/38	0/3/3/3
3	ATP	B	701	-	-	4/22/38/38	0/3/3/3
3	ATP	D	703	2	-	3/22/38/38	0/3/3/3
3	ATP	E	704	2	1/1/7/7	5/22/38/38	0/3/3/3
3	ATP	A	700	2	-	2/22/38/38	0/3/3/3
3	ATP	C	702	2	-	0/22/38/38	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	704	ATP	C5-N7	-4.43	1.31	1.39
3	C	702	ATP	C5-N7	-4.17	1.31	1.39
3	D	703	ATP	C5-N7	-4.08	1.31	1.39
3	A	700	ATP	C5-N7	-3.77	1.32	1.39
3	F	705	ATP	C5-N7	-3.73	1.32	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	704	ATP	C2'-C1'-N9	7.80	132.67	113.30
3	E	704	ATP	C4-N9-C8	-6.31	99.12	105.74
3	D	703	ATP	C4-N9-C8	-5.99	99.45	105.74
3	A	700	ATP	C2'-C1'-N9	5.86	127.87	113.30
3	D	703	ATP	O4'-C1'-N9	5.68	119.00	108.09

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	704	ATP	C1'

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	700	ATP	C5'-O5'-PA-O1A
3	E	704	ATP	C3'-C4'-C5'-O5'
3	D	703	ATP	PA-O3A-PB-O3B
3	D	703	ATP	PG-O3B-PB-O2B
3	F	705	ATP	PG-O3B-PB-O2B

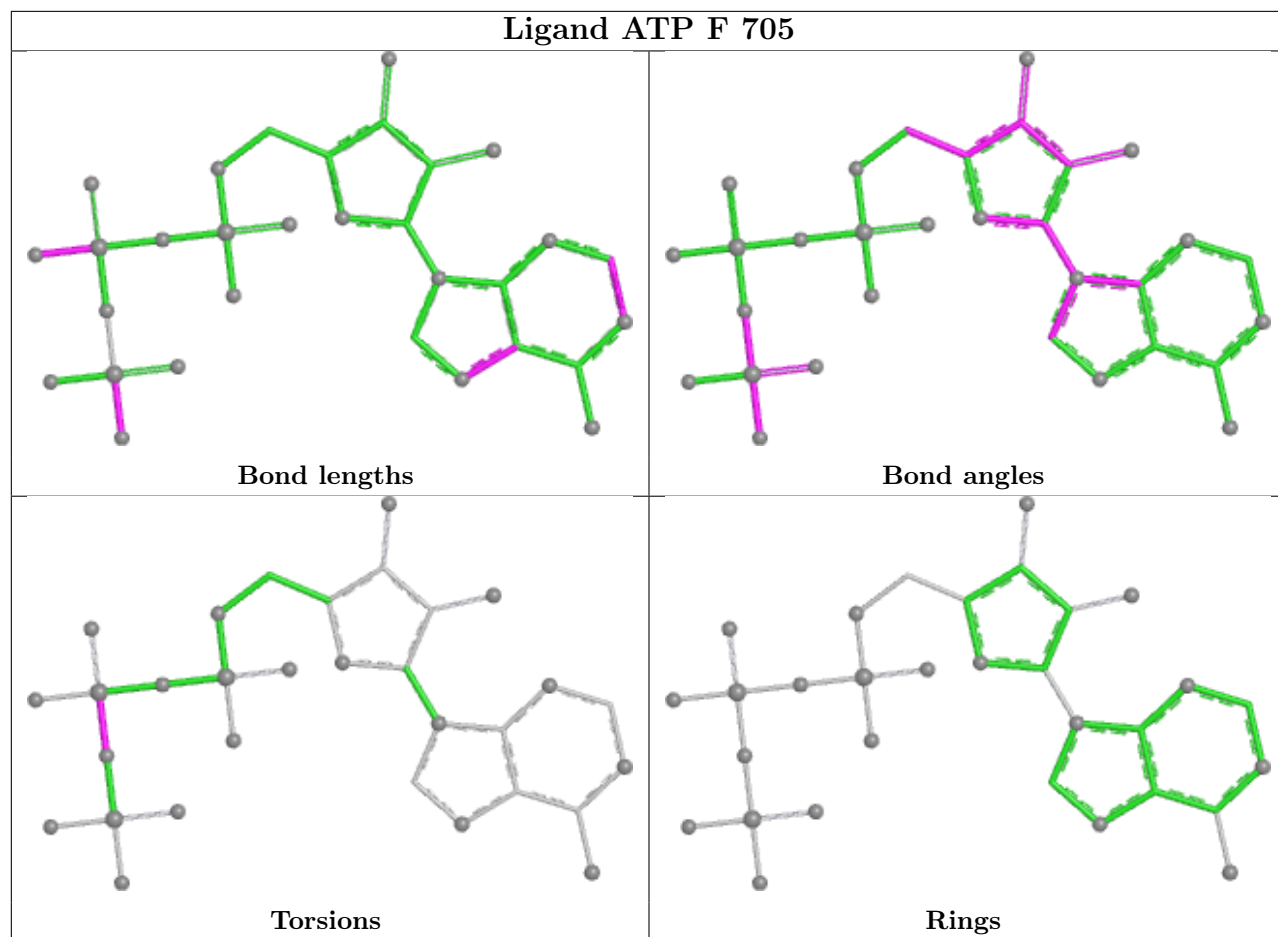
There are no ring outliers.

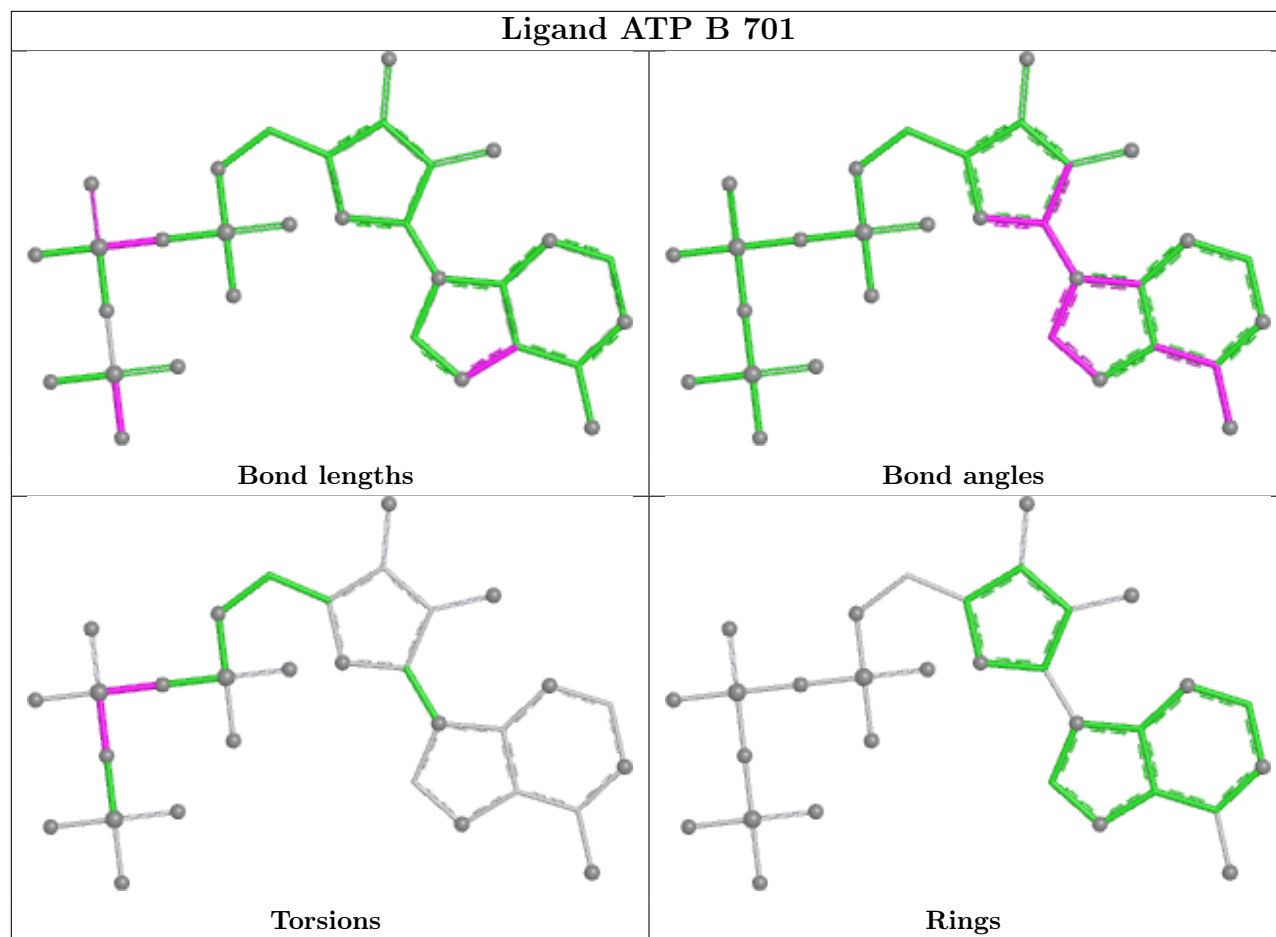
3 monomers are involved in 8 short contacts:

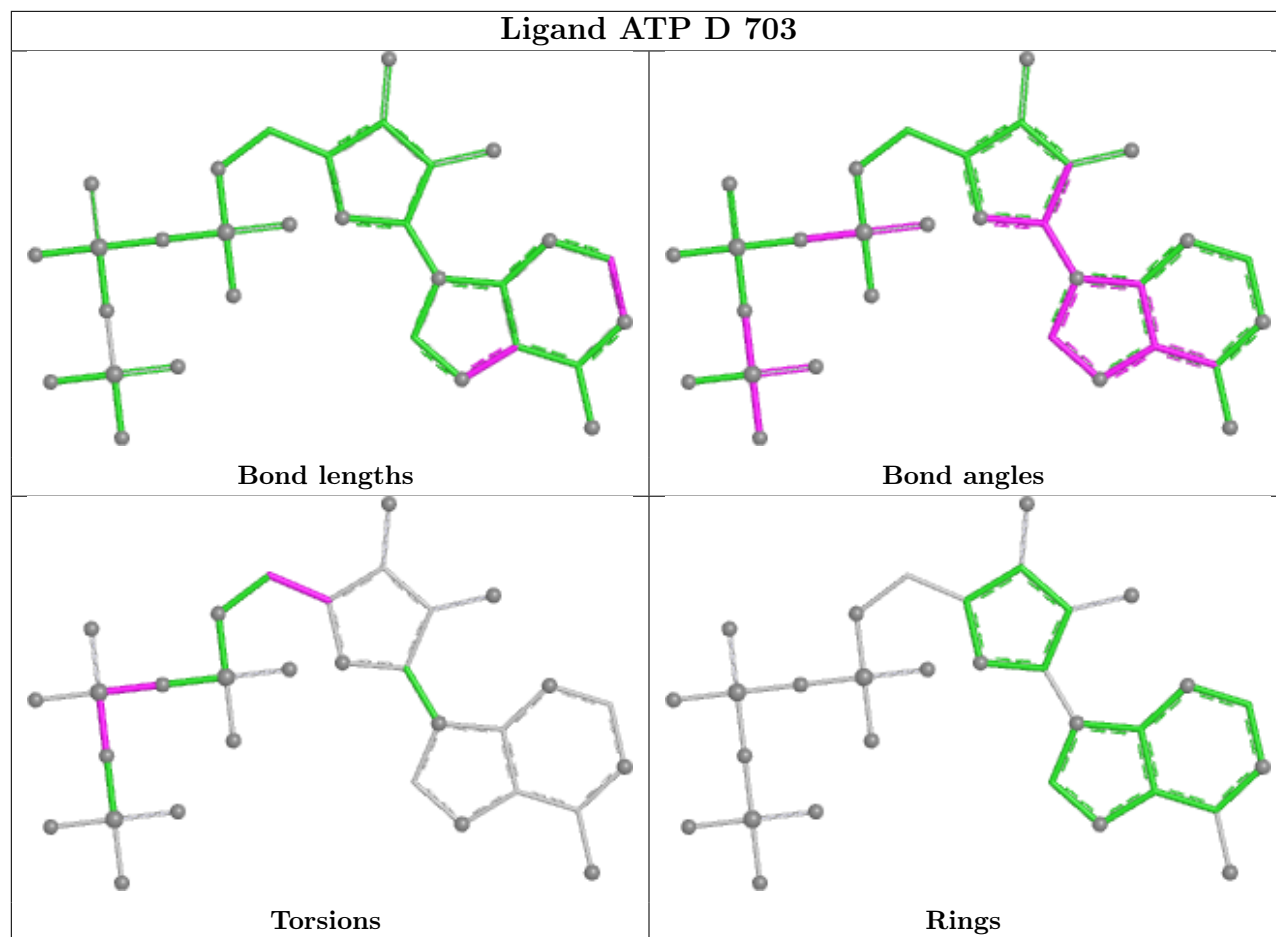
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	703	ATP	6	0
3	A	700	ATP	1	0
3	C	702	ATP	1	0

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.

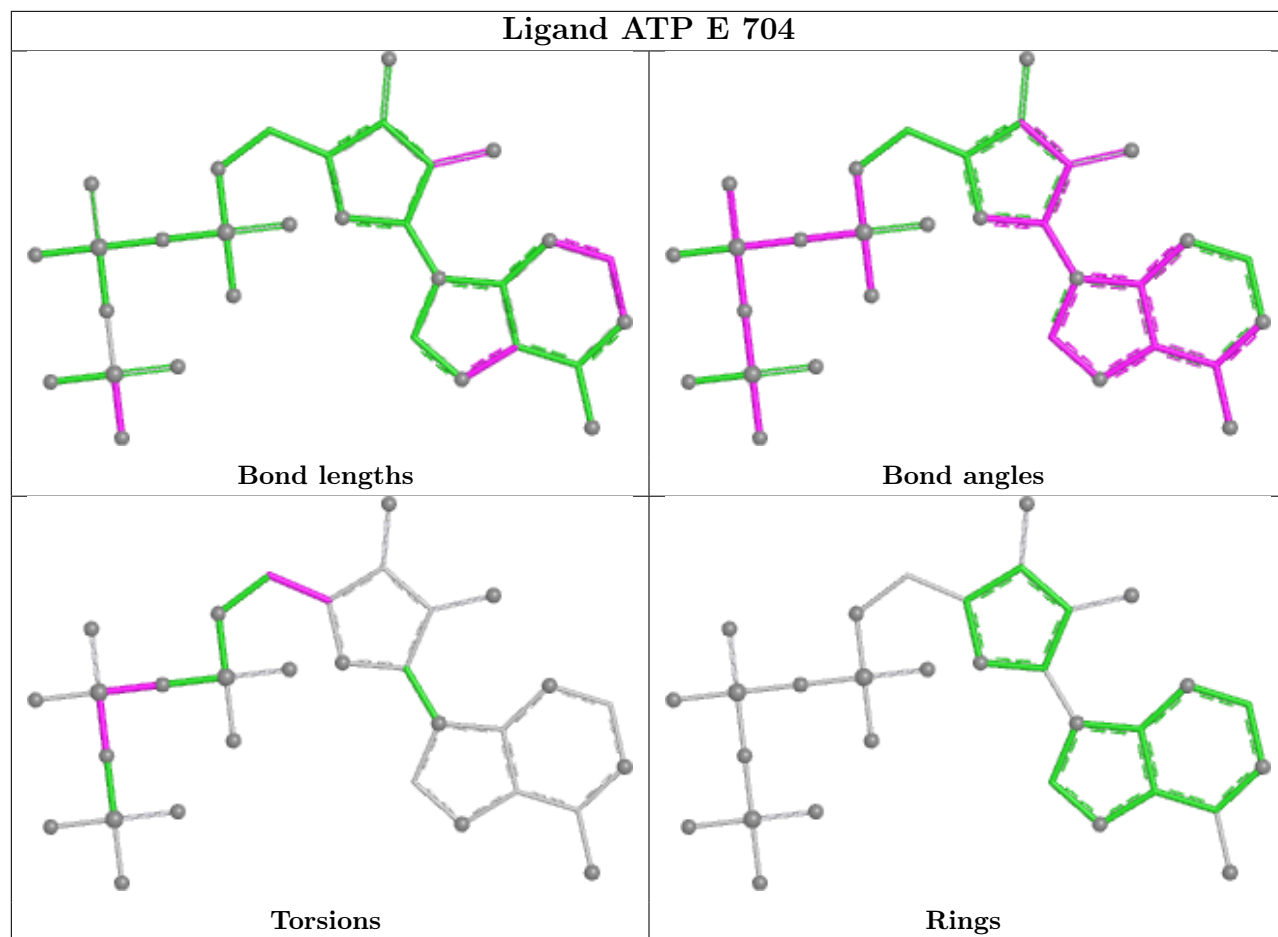
Ligand ATP F 705

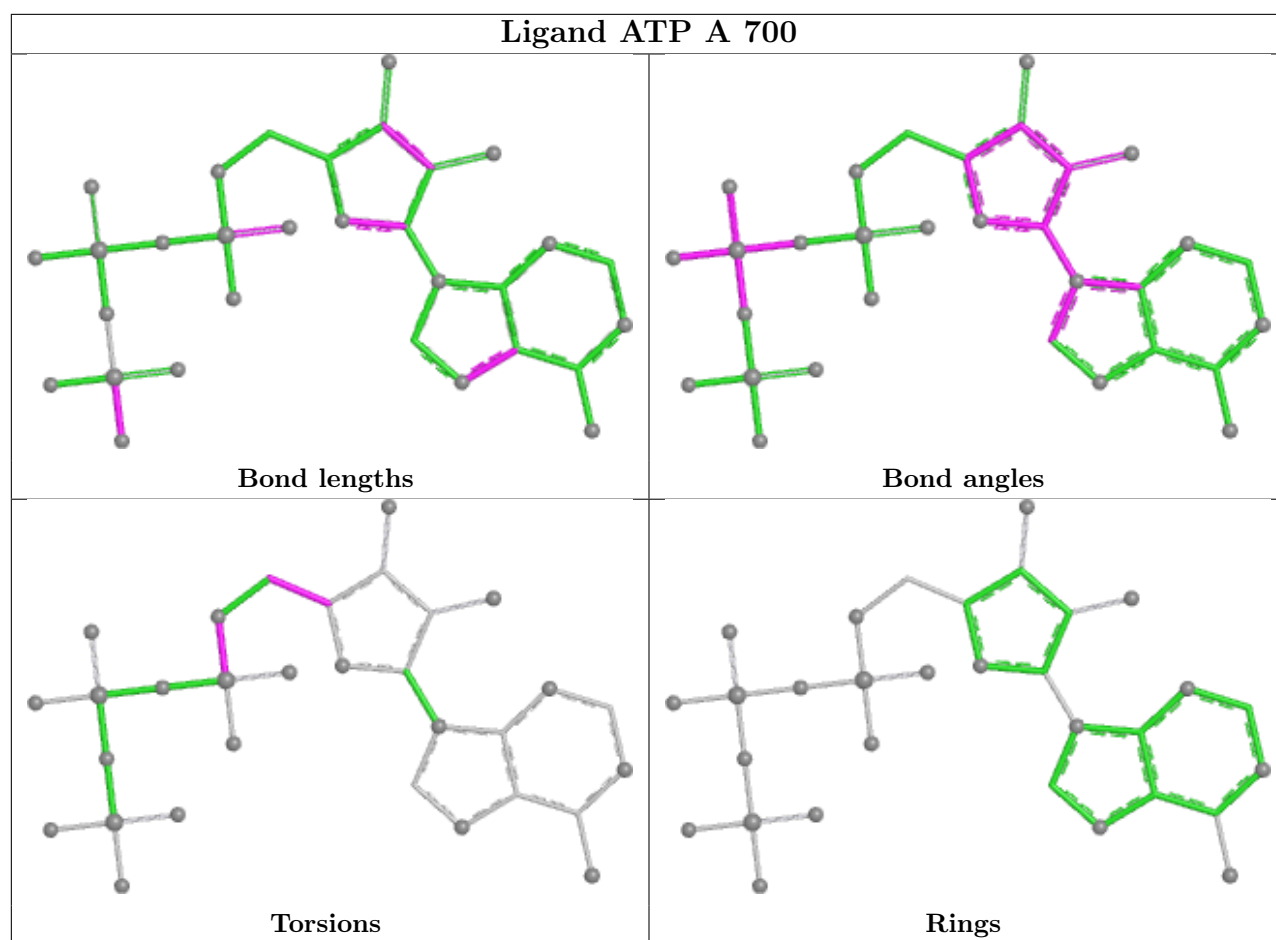


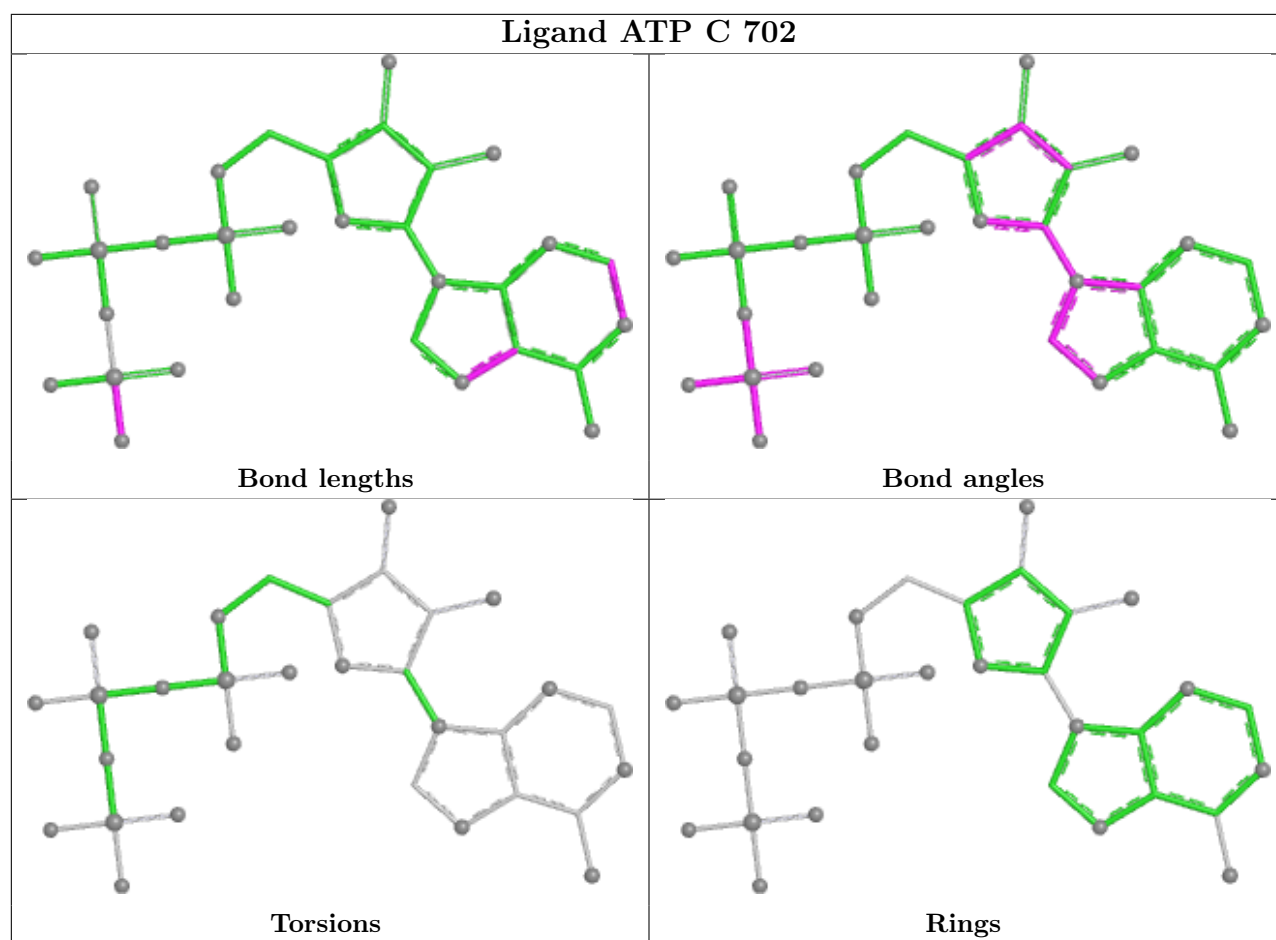




Ligand ATP E 704







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.