wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 08:48 pm BST

PDB ID	:	1JKF
Title	:	Holo 1L-myo-inositol-1-phosphate Synthase
Authors	:	Stein, A.J.; Geiger, J.H.
Deposited on	:	2001-07-12
Resolution	:	2.40 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

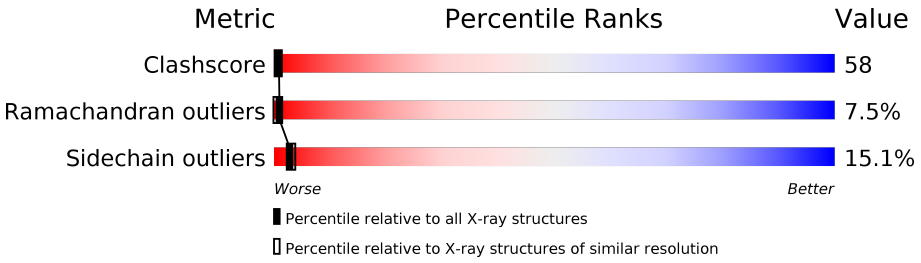
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 on 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	533	30% 43% 13% • 13%
1	B	533	25% 47% 14% • 13%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAD	B	610	-	-	X	-

2 Entry composition

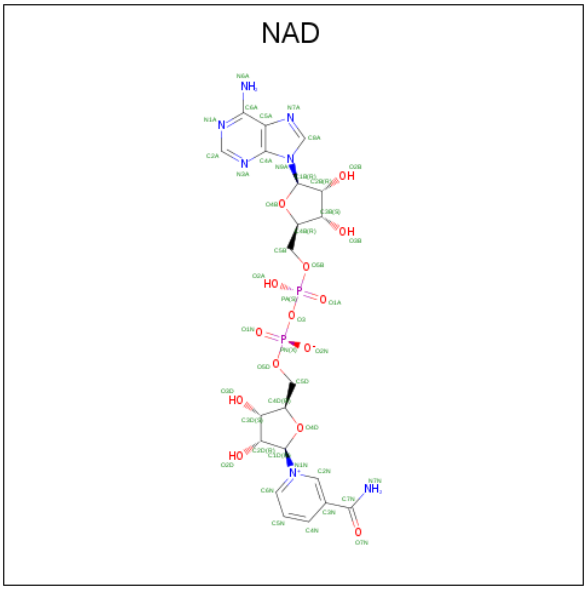
There are 3 unique types of molecules in this entry. The entry contains 7971 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 myo-inositol-1-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3675	2338	617	706	14			
1	B	465	Total	C	N	O	S	0	0	0
			3670	2336	616	704	14			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	256	Total O 256 256	0	0
3	B	282	Total O 282 282	0	0

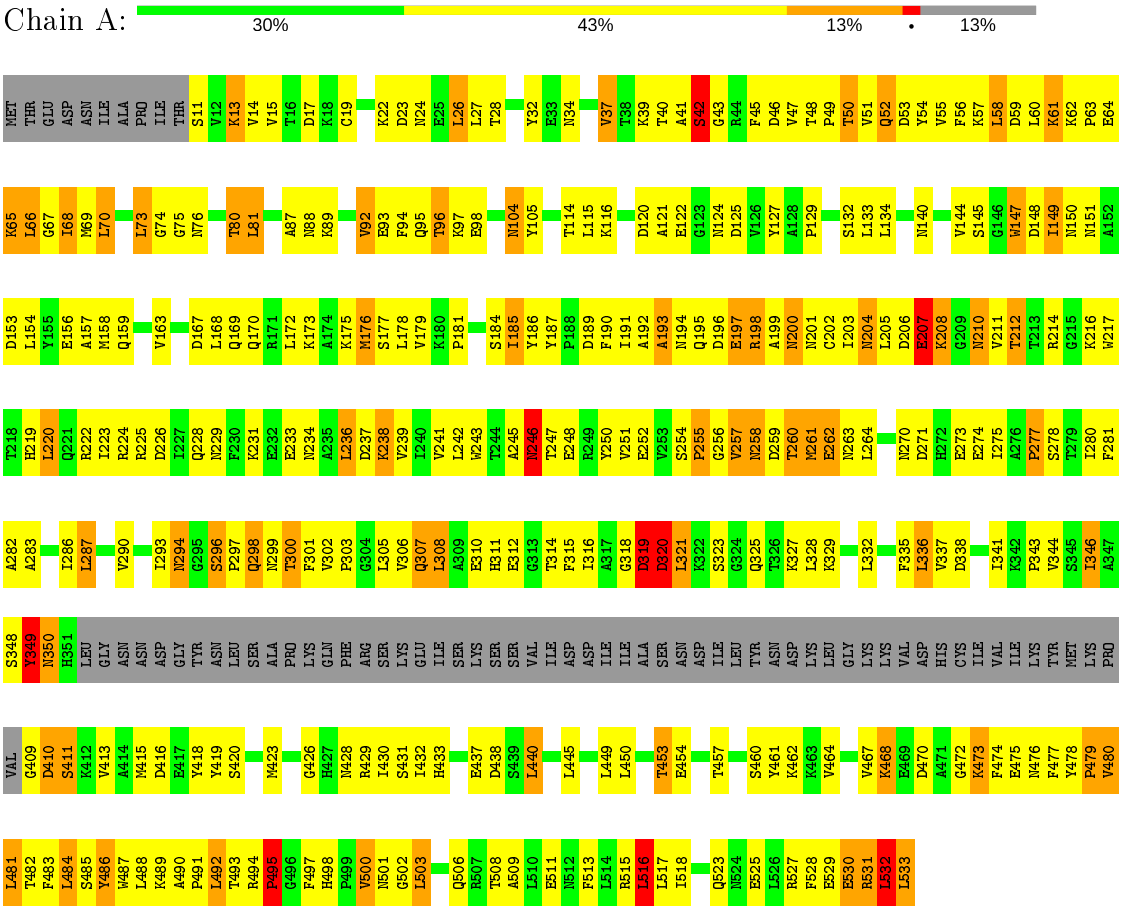
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

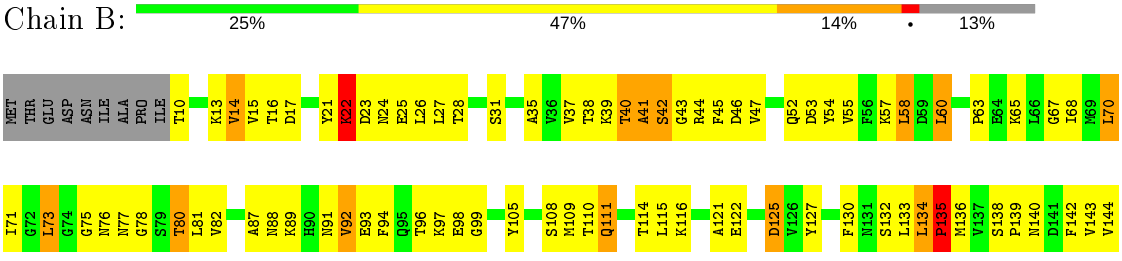
- Molecule 1: myo-inositol-1-phosphate synthase

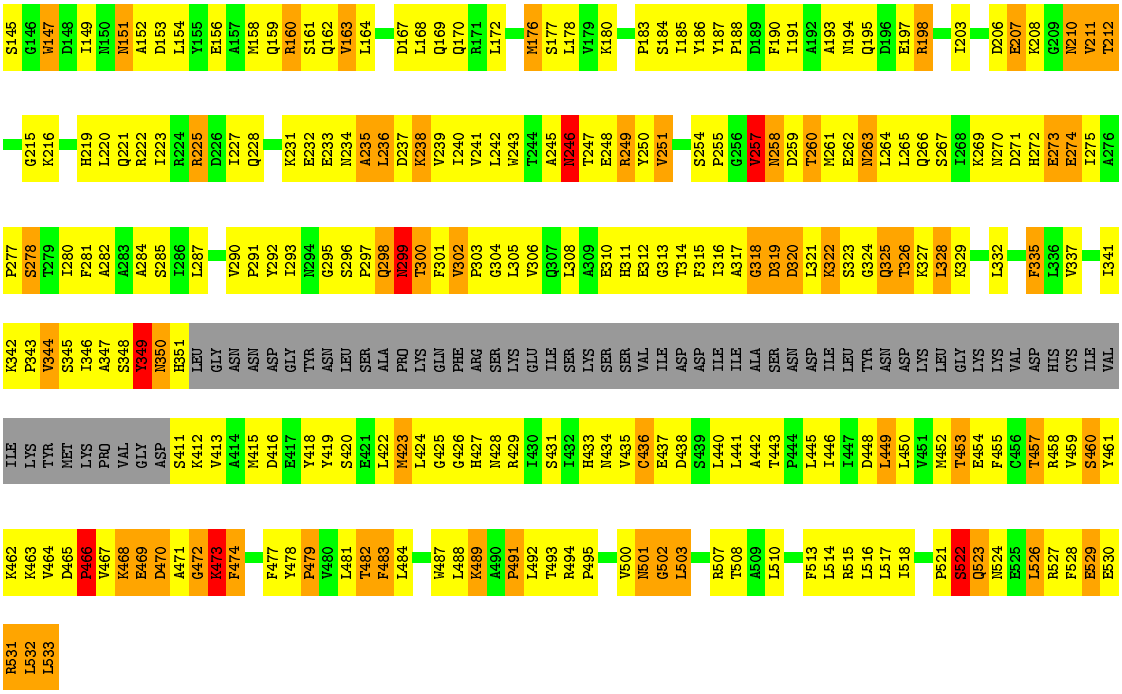
Chain A:



- Molecule 1: myo-inositol-1-phosphate synthase

Chain B:




S145 G146 W147 D148 I149 N150 N151 A152 D153 L154 Y155 E156 A157 M158 Q159 R160 S161 Q162 V163 L164 D167 L168 Q169 Q170 R171 L172 M176 S177 L178 V179 K180 P183 S184 I185 Y186 Y187 P188 D189 F190 I191 A192 A193 N194 Q195 D196 E197 R198 I203 D206 E207 K208 G209 N210 V211 T212
G215 K216 H219 L220 Q221 R222 I223 R224 R225 D226 I227 Q228 K231 E232 E233 N234 A235 L236 D237 K238 V239 I240 V241 L242 W243 T244 A245 N246 T247 E248 R249 Y250 V251 S254 P255 G256 V257 N258 D259 T260 M261 E262 N263 L264 L265 Q266 S267 I268 K269 N270 D271 H272 E273 E274 I275 A276
P277 S278 T279 I280 F281 A282 A283 A284 S285 I286 L287 V290 P291 Y292 I293 N294 G295 S296 P297 Q298 N299 T300 F301 V302 P303 G304 L305 V306 Q307 L308 A309 E310 H311 E312 G313 T314 F315 I316 A317 G318 D319 D320 L321 K322 S323 G324 Q325 T326 K327 L328 K329 L332 F335 L336 V337 I341
K342 P343 V344 S345 I346 A347 S348 Y349 N350 H351 LEU GLY ASN ASN ASP GLY TYR ASN LEU SER ALA PRO LYS GLN PHE ARG SER LYS GLU ILE SER LYS SER SER VAL ILE ASP ASP ILE ILE ALA SER ASN ASP ILE LEU TYR ASN ASP LYS LEU GLY LYS LYS VAL ASP HIS CYS ILE VAL
ILE LYS TYR MET LYS PRO VAL GLY ASP S411 K412 V413 A414 M415 D416 E417 Y418 Y419 S420 E421 L422 M423 L424 G425 G426 H427 N428 R429 I430 S431 I432 H433 N434 V435 C436 E437 D438 S439 L440 L441 A442 T443 P444 L445 I446 I447 D448 L449 L450 V451 M452 T453 E454 F455 C456 T457 R458 V459 S460 Y461
K462 K463 V464 D465 P466 V467 K468 E469 D470 A471 G472 K473 F474 F477 Y478 P479 V480 L481 T482 F483 L484 W487 L488 K489 A490 P491 L492 T493 R494 P495 V500 N501 G502 L503 R507 T508 A509 L510 F513 L514 R515 L516 L517 I518 P521 S522 Q523 N524 E525 I526 R527 F528 E529 E530
R531 L532 L533

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.04Å 95.96Å 121.29Å 90.00° 126.04° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	57.3 (10.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7971	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD

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	0.52	1/3748 (0.0%)	0.78	2/5083 (0.0%)
1	B	0.53	0/3743	0.81	3/5077 (0.1%)
All	All	0.52	1/7491 (0.0%)	0.79	5/10160 (0.0%)

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	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	MET	CG-SD	-5.11	1.67	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	318	GLY	N-CA-C	6.76	130.00	113.10
1	A	516	LEU	CA-CB-CG	6.10	129.34	115.30
1	A	73	LEU	CA-CB-CG	5.91	128.90	115.30
1	B	524	ASN	N-CA-C	-5.29	96.71	111.00
1	B	526	LEU	N-CA-C	-5.14	97.13	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	TYR	Sidechain
1	B	349	TYR	Sidechain

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	3675	0	3666	417	2
1	B	3670	0	3666	493	1
2	A	44	0	26	8	0
2	B	44	0	26	29	0
3	A	256	0	0	35	1
3	B	282	0	0	52	0
All	All	7971	0	7384	864	3

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 58.

The worst 5 of 864 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:149:ILE:HD11	1:B:195:GLN:HE21	1.04	1.13
1:B:315:PHE:HB3	1:B:481:LEU:HD11	1.30	1.12
1:B:293:ILE:HD11	1:B:453:THR:HG21	1.28	1.12
1:B:70:LEU:HD21	1:B:81:LEU:HD23	1.33	1.08
1:A:533:LEU:HG	1:B:494:ARG:HH22	0.92	1.08

All (3) 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:229:ASN:OD1	1:B:178:LEU:O[3_455]	1.70	0.50
3:A:696:HOH:O	3:A:696:HOH:O[2_555]	2.08	0.12
1:A:23:ASP:OD2	1:A:23:ASP:OD2[2_556]	2.10	0.10

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	462/533 (87%)	389 (84%)	46 (10%)	27 (6%)	1 0
1	B	461/533 (86%)	360 (78%)	59 (13%)	42 (9%)	1 0
All	All	923/1066 (87%)	749 (81%)	105 (11%)	69 (8%)	1 0

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	VAL
1	A	207	GLU
1	A	298	GLN
1	A	319	ASP
1	B	22	LYS

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	410/471 (87%)	348 (85%)	62 (15%)	3 3
1	B	410/471 (87%)	348 (85%)	62 (15%)	3 3
All	All	820/942 (87%)	696 (85%)	124 (15%)	3 3

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	HIS

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Mol	Chain	Res	Type
1	B	80	THR
1	B	473	LYS
1	A	500	VAL
1	B	14	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	476	ASN
1	B	24	ASN
1	B	307	GLN
1	A	501	ASN
1	A	504	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)

2 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	NAD	B	610	-	42,48,48	2.80	16 (38%)	50,73,73	1.40	6 (12%)
2	NAD	A	600	1	42,48,48	2.68	13 (30%)	50,73,73	1.40	6 (12%)

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	NAD	B	610	-	-	7/26/62/62	0/5/5/5
2	NAD	A	600	1	-	10/26/62/62	0/5/5/5

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	610	NAD	C4N-C3N	9.10	1.54	1.39
2	A	600	NAD	C4N-C3N	8.54	1.53	1.39
2	B	610	NAD	C2A-N1A	6.75	1.46	1.33
2	A	600	NAD	C2N-C3N	5.97	1.48	1.39
2	A	600	NAD	C6N-N1N	5.91	1.49	1.35

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	610	NAD	C3N-C7N-N7N	4.45	123.09	117.75
2	A	600	NAD	C3N-C7N-N7N	4.13	122.70	117.75
2	A	600	NAD	C3D-C2D-C1D	3.79	106.69	100.98
2	A	600	NAD	O4B-C1B-C2B	-2.96	102.60	106.93
2	A	600	NAD	N3A-C2A-N1A	-2.95	124.07	128.68

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	610	NAD	O4B-C4B-C5B-O5B
2	B	610	NAD	O4D-C4D-C5D-O5D
2	A	600	NAD	C5D-O5D-PN-O3
2	A	600	NAD	C5D-O5D-PN-O2N
2	A	600	NAD	O4D-C4D-C5D-O5D

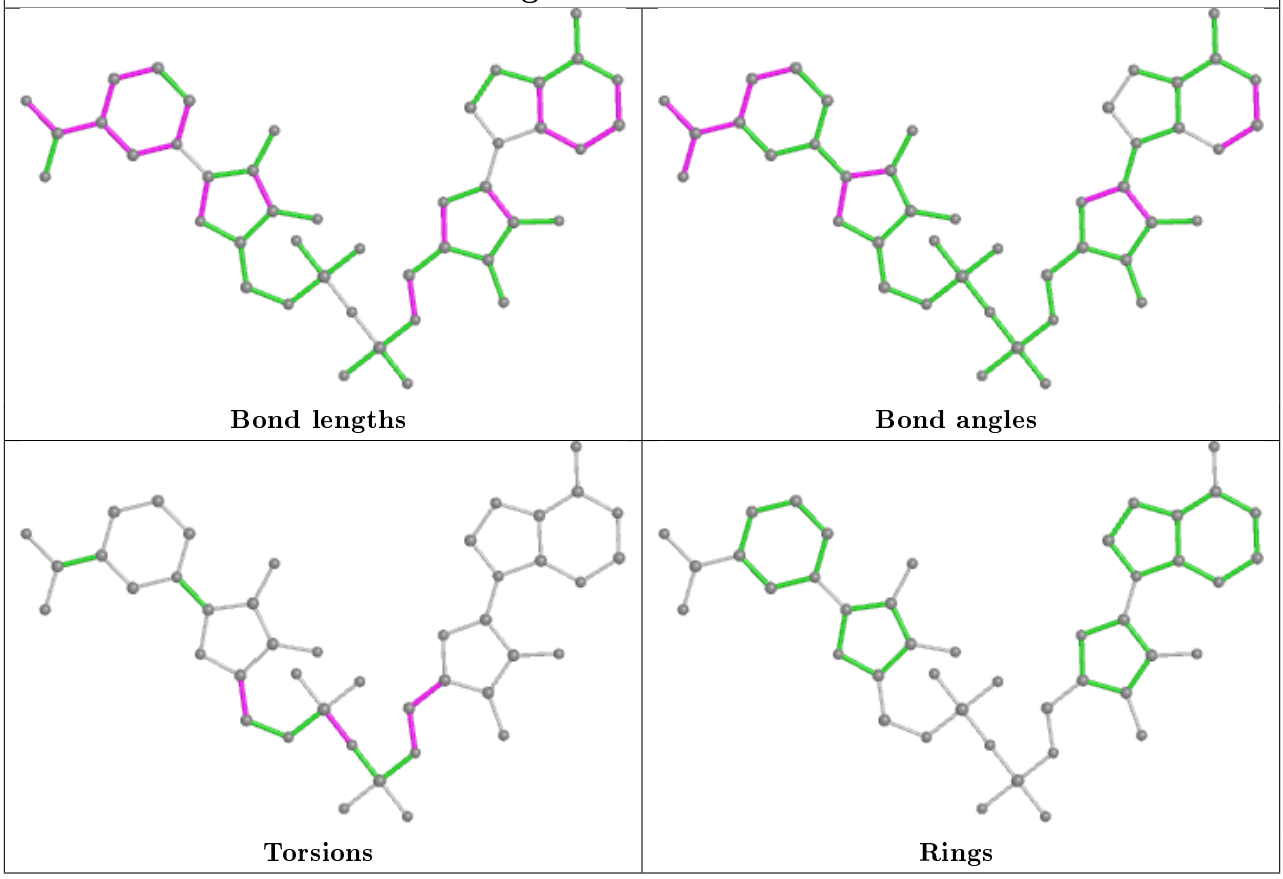
There are no ring outliers.

2 monomers are involved in 37 short contacts:

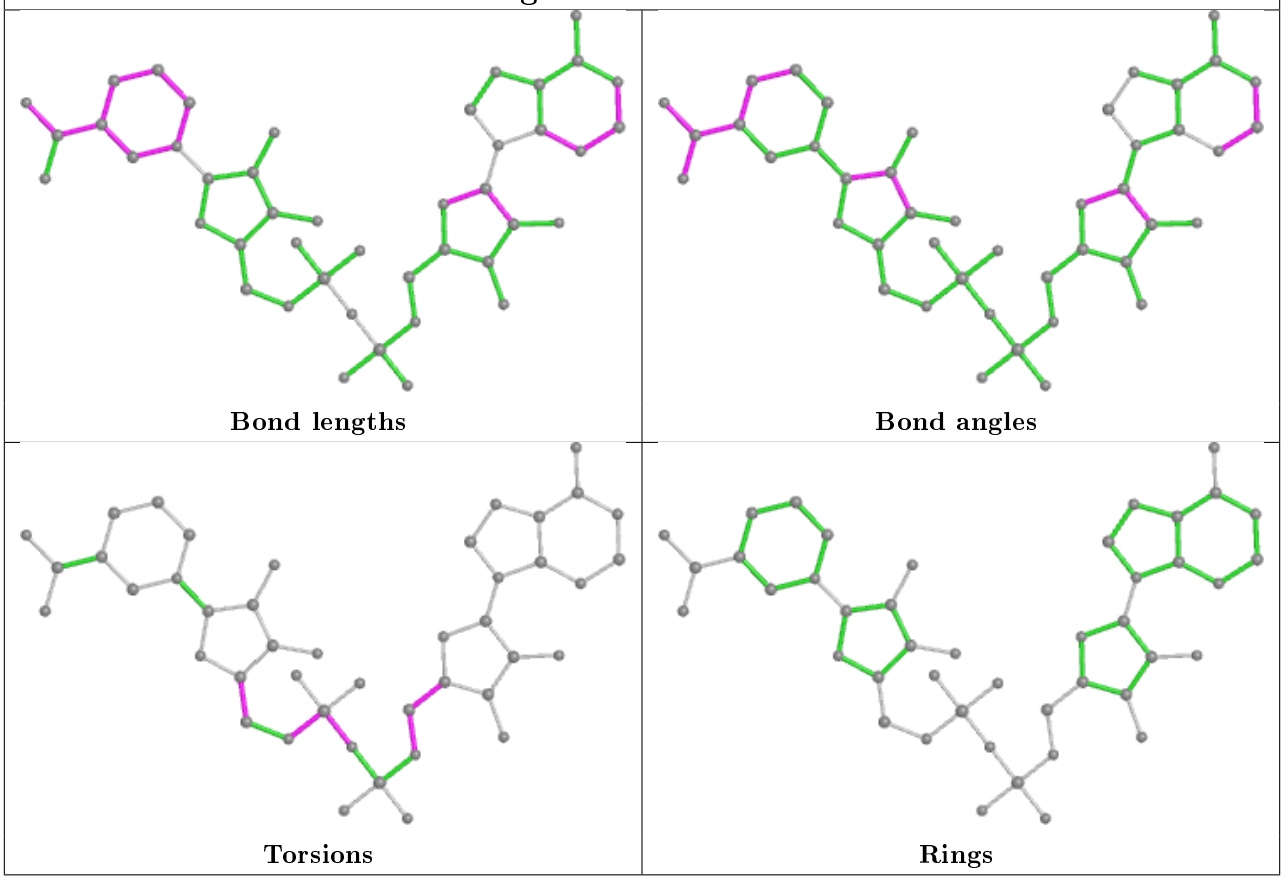
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	610	NAD	29	0
2	A	600	NAD	8	0

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 then 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 NAD B 610



Ligand NAD A 600



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.