



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 08:34 am BST

PDB ID : 1JKI  
Title : myo-Inositol-1-phosphate Synthase Complexed with an Inhibitor, 2-deoxy-glucitol-6-phosphate  
Authors : Stein, A.J.; Geiger, J.H.  
Deposited on : 2001-07-12  
Resolution : 2.20 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.

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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)
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

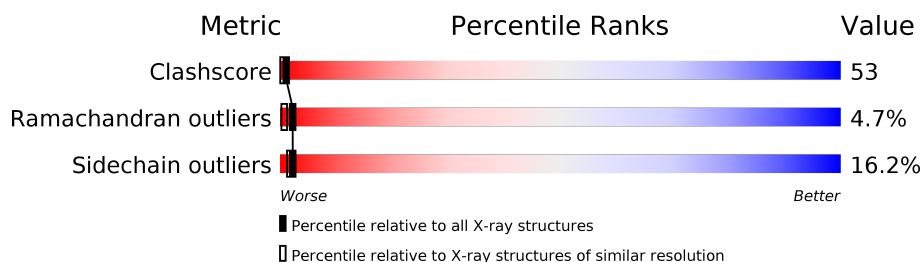
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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  $\geq 3$ , 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	533	
1	B	533	

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
3	DG6	A	630	X	X	X	-
3	DG6	B	640	X	X	X	-

## 2 Entry composition [i](#)

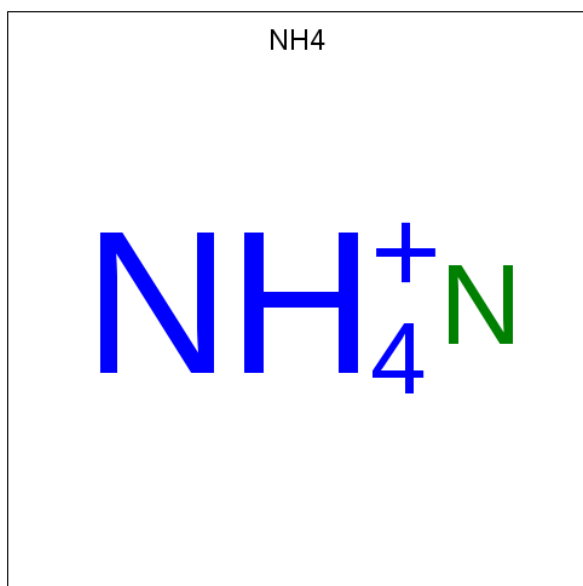
There are 5 unique types of molecules in this entry. The entry contains 9006 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

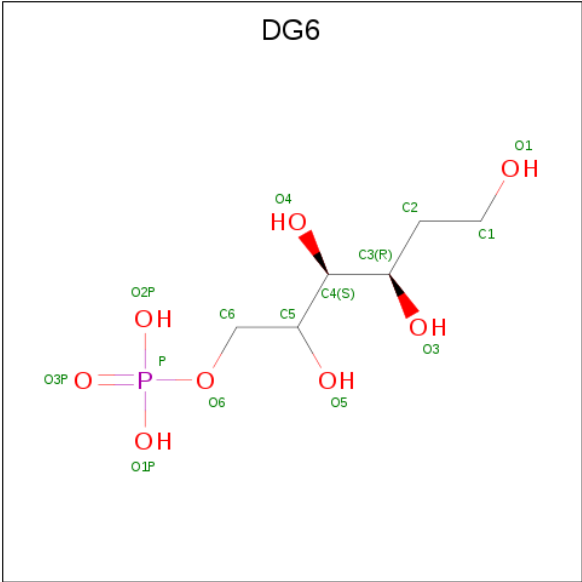
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4138	2632	695	795	16			
1	B	524	Total	C	N	O	S	0	0	0
			4130	2626	694	794	16			

- Molecule 2 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N).



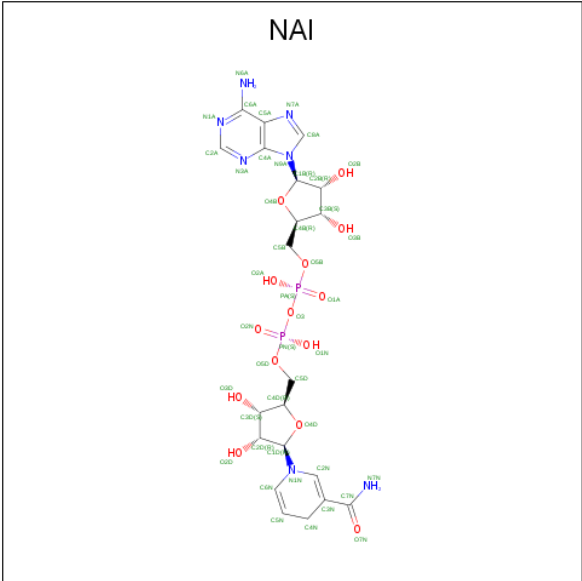
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N	0	0
			1	1		
2	B	1	Total	N	0	0
			1	1		

- Molecule 3 is 2-DEOXY-GLUCITOL-6-PHOSPHATE (three-letter code: DG6) (formula: C<sub>6</sub>H<sub>15</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			15	6	8	1		
3	B	1	Total	C	O	P	0	0
			15	6	8	1		

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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

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

- Molecule 5 is water.

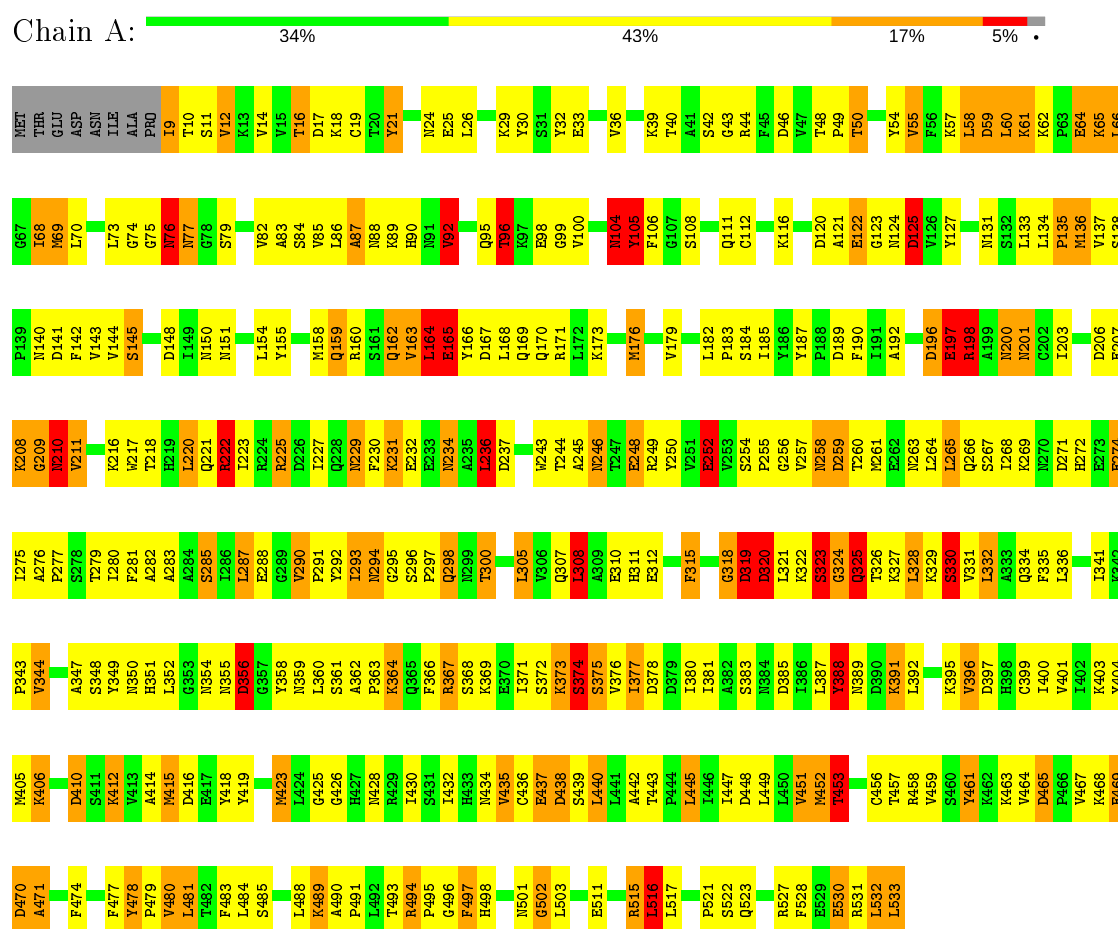
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total	O	0	0
			303	303		
5	B	315	Total	O	0	0
			315	315		

### 3 Residue-property plots

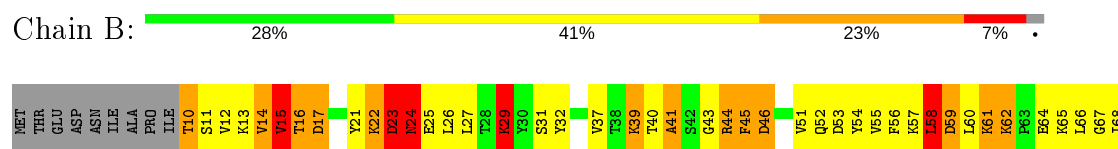
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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



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



L481	A414	A347	M415	S348	A282	K208	N140	M69
T482	M416	S349	Y349	N350	I286	G209	D141	L70
F483	D416	Y349	N350	H351	L287	N210	F142	I71
L484	E417	H351	H351	R351	E288	V211	V143	G72
S485	Y418	L352	G353	L352	Q289	T212	Y144	L73
Y486	Y419	G353	N354	N355	V290	T213	W147	G74
W487	M423	N354	N355	D356	P291	K216	G75	N76
L488	L488	N354	N355	G357	Y292	W217	I149	
A490	G426	N355	N355	H358	I293	T218	N150	S79
P491	H427	G357	G358	N359	G295	H219	M151	T80
L492	H428	N358	N358	L360	I294	R222	A152	L81
T493	H429	N359	N359	S296	G295	I223	D153	V82
R494	I430	L360	L360	S296	S296	I223	L154	A83
P495	S431	S361	S361	A362	P297	R224	S84	S84
G496		A362	A362	Q298	R225	R225	Y155	V85
F497	C436	P363	P363	N299	Q228	Q228	M158	L86
H498	E437	K364	K364		N229	N229	Q159	A87
P499	D438	Q365	Q365	V302	F230	F230	R160	
V500	S439	F366	F366	P303	R231	R231	S161	V92
N501	L440	R367	R367	G304	K231	K231	Q162	E93
G502	L441	S368	S368	L305	E232	E232	V163	F94
L503	A442	K369	K369	V306	E233	E233	L164	Q95
N504	T443	E370	E370	Q307	Q236	Q236	E165	T96
K505	P444	I371	I371	L308	D237	D237	Y166	K97
Q506	L445	S372	S372	A309	K237	K237	D167	
R507	I446	K373	K373	E310	L242	L242	L168	K101
	I447	S374	S374	H311	V239	V239	Q169	Q102
	D448	S375	S375		I240	I240	Q170	P103
L510	L449	V376	V376	T314	V241	V241	A171	N104
E511	L450	I377	I377	F315	L243	L243	L172	Y105
	V451	D378	D378	I316	T244	T244	K173	F106
R515	M452	D379	D379	G318	A245	A245	G107	S108
L516	T453	I380	I380	D319	N246	N246	M176	S108
L517	E454				T247	T247	S177	M109
F455	F455	D385	D385	D320	E248	E248	L178	
G456	G456	I386	I386	L321	R249	R249	V179	S113
T457	L520	V387	V387	S323	Y250	Y250	T114	T114
R458	P521	Y388	Y388	S323	E251	E251	L115	L115
S522	V459			G324	E252	E252	I185	K116
Q523	S460	L392	L392	Q325	V253	V253	Y186	
N524	Y461			T326			Y187	I119
E525	E462	K395	K395	K327	S254	S254	F190	E122
L526	K463	V396	V396	L328	P255	P255	I191	G123
R527	V464	D397	D397	K329	G256	G256	A192	G123
F528	D465	H398	H398	S330	V257	V257	A192	N124
E529	P466	G399	G399	V331	N258	N258	A193	D125
E530	V467	I400	I400	L332	D259	D259	N194	V126
	K468	V401	V401	R332	T260	T260	Q195	
R531	E469	I402	I402	A333	M261	M261	D196	P129
L532	D470	K403	K403	Q334	E197	E197	F130	F130
	G471	Y404	Y404	F335	L264	L264	N131	S132
G472	K473	M405	M405	P337	L265	L265	A199	L133
K473	F474	K406	K406	D338	E273	E273	N200	L134
	V474	V408	V408		E274	E274	N201	L134
	F477			K342	P343	P343	P135	P135
L533	F477	S411	S411	V344	I275	I275	M136	
	Y478	K412	K412	V345	S277	S277	L205	V137
	V479	V479	V479	I246	S578	S578	D206	S138
							E507	P139

## 4 Data and refinement statistics

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, $\alpha$ , $\beta$ , $\gamma$	152.73Å 98.31Å 121.86Å 90.00° 126.09° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	87.6 (10.00-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.208 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9006	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	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: NH4, NAI, DG6

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	1.87	91/4219 (2.2%)	1.52	58/5719 (1.0%)
1	B	1.95	97/4211 (2.3%)	1.69	81/5708 (1.4%)
All	All	1.91	188/8430 (2.2%)	1.61	139/11427 (1.2%)

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	0	7
All	All	0	12

The worst 5 of 188 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	MET	CB-CG	9.86	1.82	1.51
1	A	165	GLU	CB-CG	9.64	1.70	1.52
1	A	32	TYR	CE1-CZ	8.97	1.50	1.38
1	A	356	ASP	CB-CG	8.89	1.70	1.51
1	A	388	TYR	CE1-CZ	8.76	1.50	1.38

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ARG	NE-CZ-NH2	-21.35	109.62	120.30
1	B	222	ARG	NE-CZ-NH1	18.52	129.56	120.30
1	B	321	LEU	CB-CG-CD2	-13.96	87.26	111.00
1	A	423	MET	CG-SD-CE	13.56	121.90	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	ASP	CB-CG-OD2	11.97	129.07	118.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	TYR	Sidechain
1	A	21	TYR	Sidechain
1	A	388	TYR	Sidechain
1	A	461	TYR	Sidechain
1	A	478	TYR	Sidechain

## 5.2 Too-close contacts

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	4138	0	4147	420	1
1	B	4130	0	4136	505	0
2	A	1	0	0	1	0
2	B	1	0	0	1	0
3	A	15	0	12	10	0
3	B	15	0	12	17	0
4	A	44	0	22	8	0
4	B	44	0	24	3	0
5	A	303	0	0	55	0
5	B	315	0	0	63	0
All	All	9006	0	8353	891	1

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 53.

The worst 5 of 891 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:69:MET:CB	1:B:69:MET:CG	1.82	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:MET:SD	1:A:136:MET:CG	2.02	1.46
1:B:69:MET:CE	1:B:69:MET:SD	2.08	1.40
1:A:415:MET:CE	1:A:415:MET:SD	2.09	1.40
1:A:69:MET:SD	1:A:69:MET:CE	2.13	1.36

All (1) 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:415:MET:CE	1:A:415:MET:CE[2_555]	2.03	0.17

## 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	523/533 (98%)	463 (88%)	37 (7%)	23 (4%)	2	1
1	B	522/533 (98%)	444 (85%)	52 (10%)	26 (5%)	2	0
All	All	1045/1066 (98%)	907 (87%)	89 (8%)	49 (5%)	2	1

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLY
1	A	197	GLU
1	A	198	ARG
1	A	208	LYS
1	A	210	ASN

### 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	464/471 (98%)	396 (85%)	68 (15%)	3	2
1	B	463/471 (98%)	381 (82%)	82 (18%)	2	1
All	All	927/942 (98%)	777 (84%)	150 (16%)	2	2

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	533	LEU
1	B	129	PRO
1	B	484	LEU
1	B	15	VAL
1	B	61	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
1	A	523	GLN
1	B	428	ASN
1	A	350	ASN
1	A	428	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are modelled with single atom - 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	NAI	A	650	-	42,48,48	3.79	26 (61%)	47,73,73	2.38	15 (31%)
3	DG6	A	630	-	14,14,14	4.56	10 (71%)	18,19,19	2.44	5 (27%)
4	NAI	B	660	-	42,48,48	3.91	25 (59%)	47,73,73	2.42	20 (42%)
3	DG6	B	640	-	14,14,14	3.87	8 (57%)	18,19,19	2.22	6 (33%)

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	NAI	A	650	-	-	8/25/72/72	0/5/5/5
3	DG6	A	630	-	1/1/4/4	10/17/17/17	-
4	NAI	B	660	-	-	4/25/72/72	0/5/5/5
3	DG6	B	640	-	1/1/4/4	8/17/17/17	-

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	660	NAI	O4B-C1B	-11.54	1.25	1.41
4	B	660	NAI	C4A-N3A	10.81	1.50	1.35
3	A	630	DG6	C6-C5	9.39	1.65	1.51
3	B	640	DG6	C6-C5	8.92	1.64	1.51
4	A	650	NAI	O2B-C2B	-8.36	1.23	1.43

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	650	NAI	O4D-C1D-N1N	7.65	123.00	108.06
4	A	650	NAI	O2A-PA-O1A	5.95	141.64	112.24
4	B	660	NAI	O4D-C1D-N1N	5.50	118.82	108.06
3	A	630	DG6	C6-C5-C4	5.46	122.75	112.20
4	A	650	NAI	O7N-C7N-N7N	-5.31	110.45	122.88

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	640	DG6	C5
3	A	630	DG6	C5

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	640	DG6	O1-C1-C2-C3
3	B	640	DG6	C2-C3-C4-O4
3	B	640	DG6	O3-C3-C4-O4
3	B	640	DG6	O3-C3-C4-C5
3	B	640	DG6	C3-C4-C5-O5

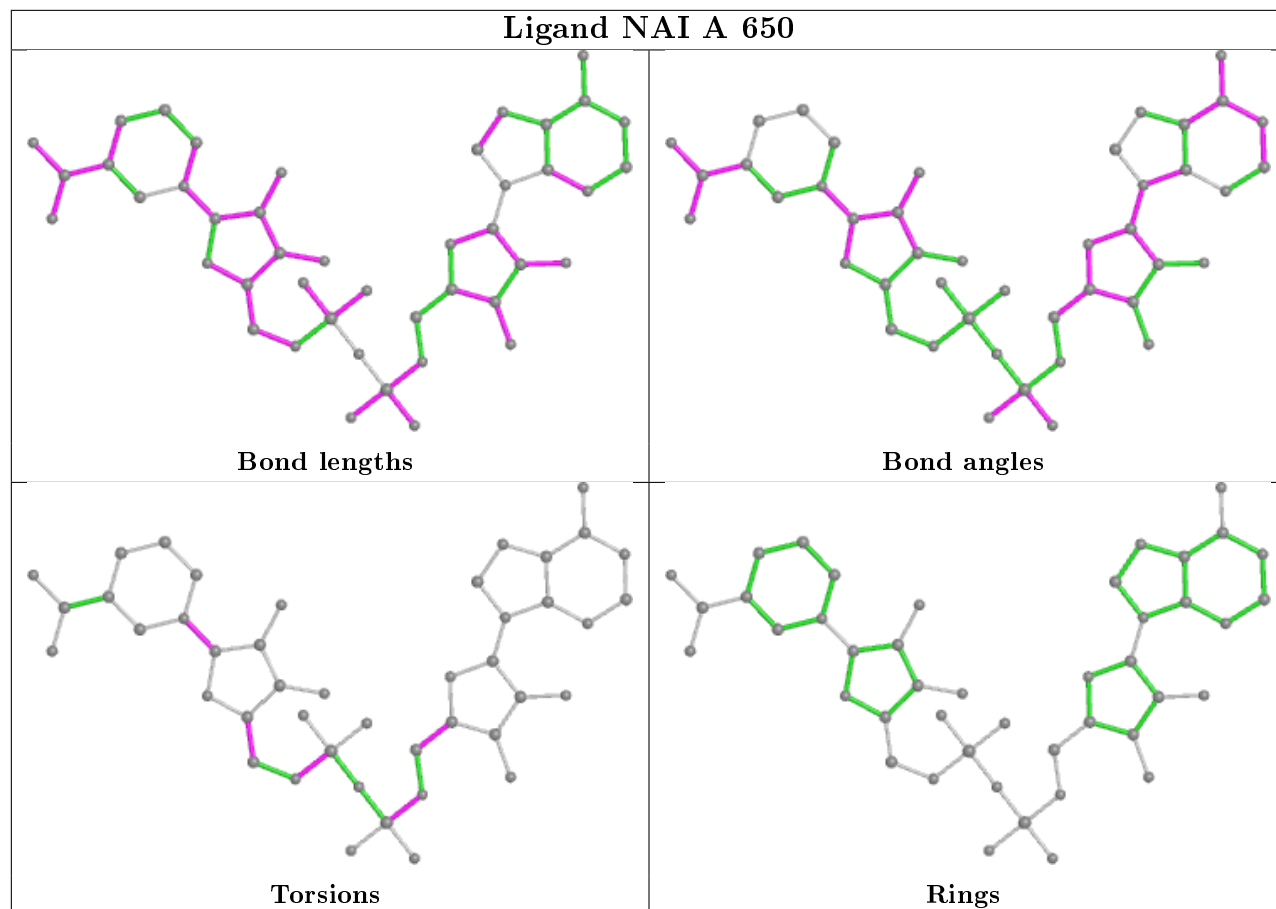
There are no ring outliers.

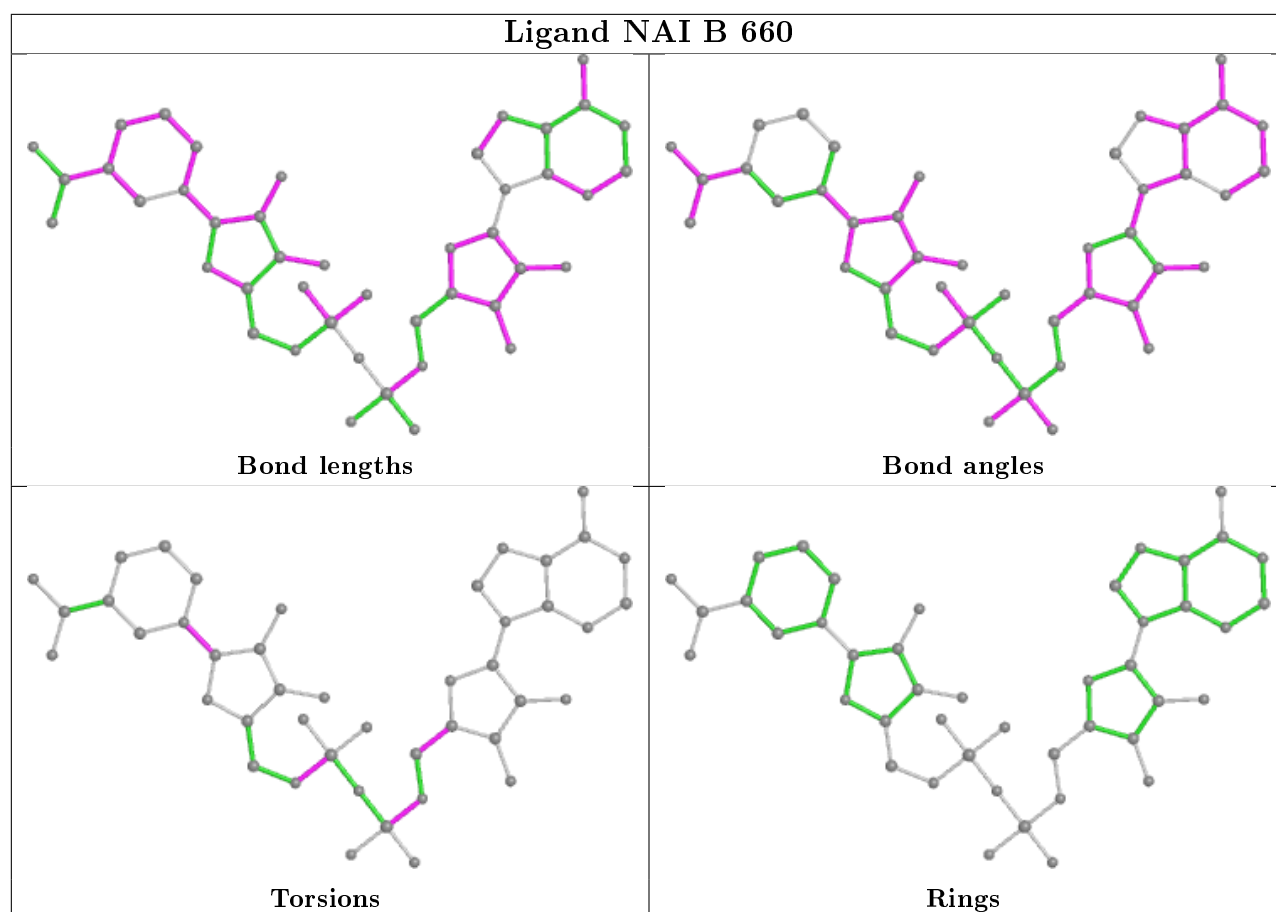
4 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	650	NAI	8	0
3	A	630	DG6	10	0
4	B	660	NAI	3	0
3	B	640	DG6	17	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 [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.