



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 11:13 PM UTC

PDB ID : 1JKI / pdb_00001jki
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

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

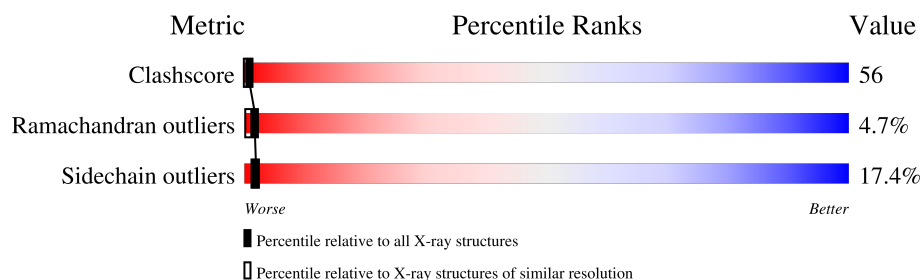
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 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	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](#)

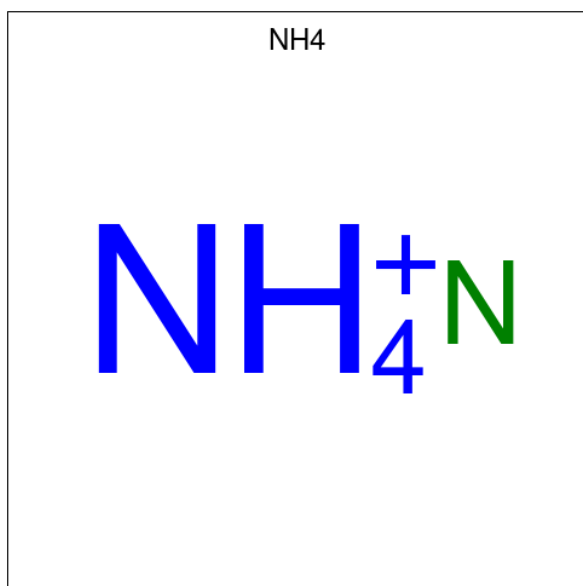
There are 5 unique types of molecules in this entry. The entry contains 9006 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

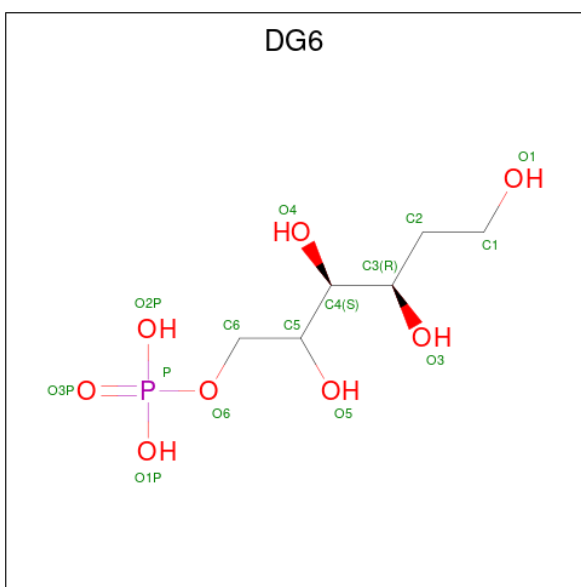
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4138	2632	695	795	16			
1	B	524	Total	C	N	O	S	0	0	0
			4130	2626	694	794	16			

- Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula: H_4N).



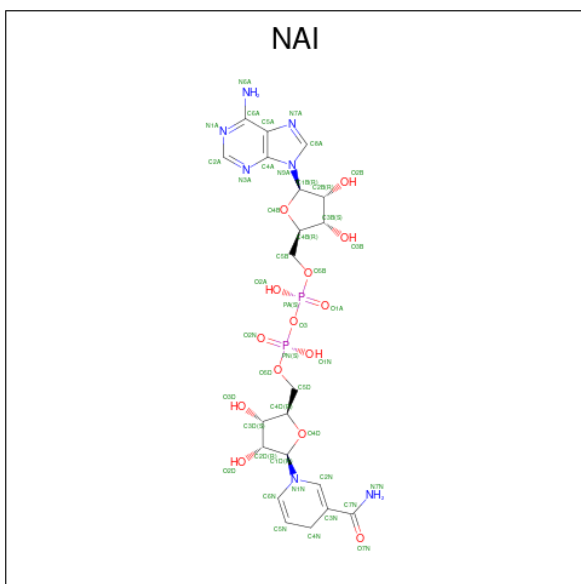
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N	0	0
			1	1		
2	B	1	Total	N	0	0
			1	1		

- Molecule 3 is 2-DEOXY-GLUCITOL-6-PHOSPHATE (CCD ID: DG6) (formula: $\text{C}_6\text{H}_{15}\text{O}_8\text{P}$).



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

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



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

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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.

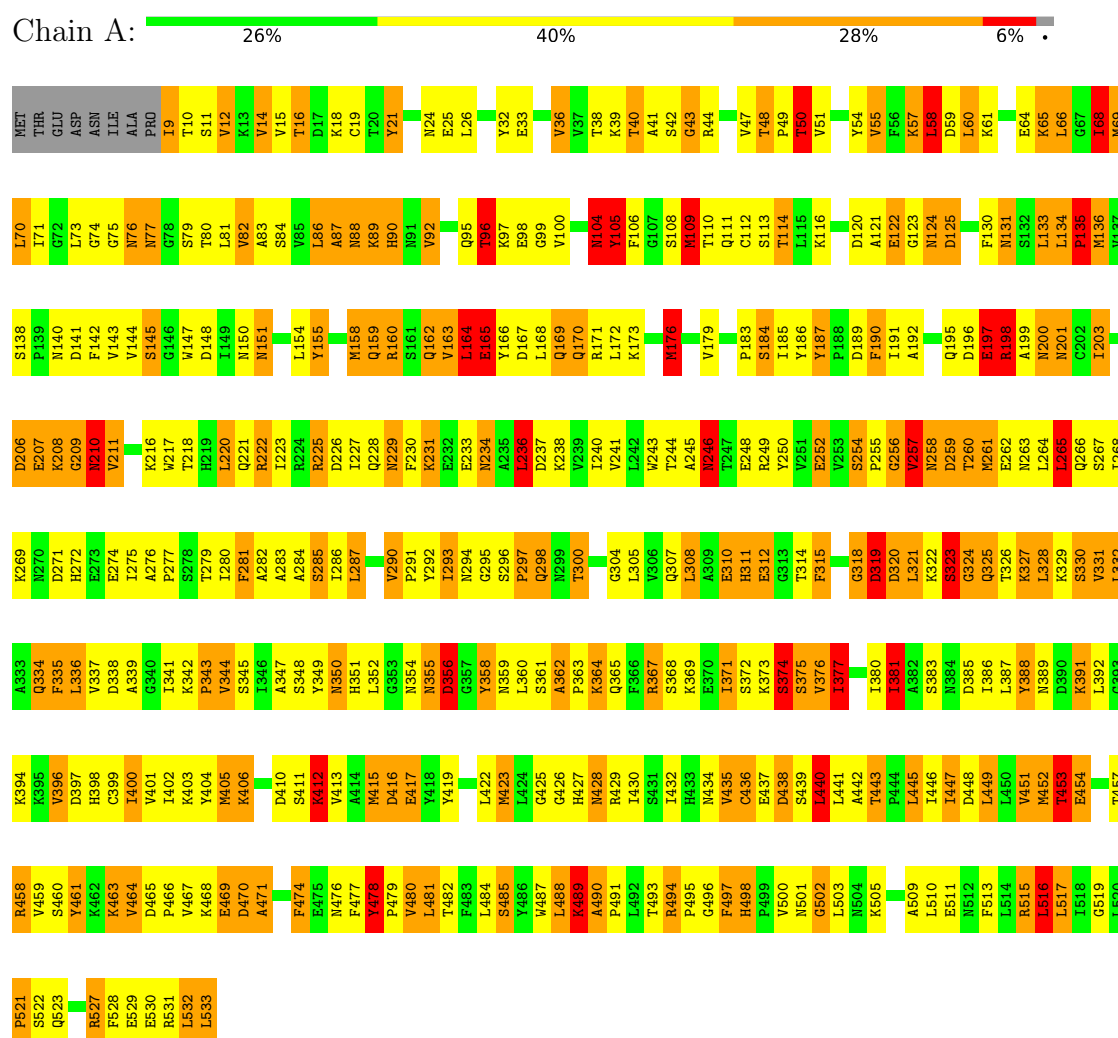
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total	O	0	0
			303	303		
5	B	315	Total	O	0	0
			315	315		

3 Residue-property plots

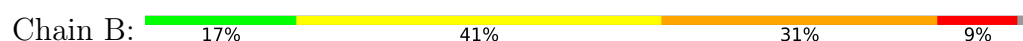
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: myo-inositol-1-phosphate synthase



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



L503	A442	D379	I316	R249	N124	K62	MET
M504	T443	I380	A317	Y250	D125	P63	THR
Q506	P444	I381	G318	V251	A128	P64	GLU
R507	L445	A382	D319	E252	F190	K65	ASP
	I446	S383	D320	F191	I191	L66	ASN
L510	T447	R384	L321	S254	A192	G67	ILE
D448	D385	D385	K322	P255	A193	I68	ALA
L449	I386	I386	G324	G256	N131	M69	PRO
L450	L387	L387	S323	V257	L133	L70	ILE
V451	Y388	Y388	G324	N258	L134	I71	T10
M452			T326	D259	P135	G72	S11
T453	K391	K391	K327	T260	M136	L73	V12
E454	L392	L392	L328	M261	V137	G74	K13
F455			K329	N200	S138	G75	V14
C456	K396	K396	S330	N201	P139	N76	V15
T457	V396	V396	V331	C202	N140	N77	T16
R458	D397	D397	L332	I203	N141	G78	D17
V459	H398	H398	A333	N204	F142	S79	K18
S460	C399	C399	Q334	L205	V143	T80	C19
Y461	I400	I400	F335	D206	V144	L81	T20
K462	V401	V401	E273	E207	S145	V82	Y21
R463	T402	T402	E274	K208	G146	V82	Y21
V464	K403	K403	I275	G209	W147	S84	D22
D465	Y404	Y404	A276	N210	D148	V85	N24
P466	M405	M405	P277	V211	I149	L86	E25
V467	K406	K406	S278	T212	N150	A87	L26
K468	P407	P407	T279	T213	M151	N88	L27
E469	V408	V408	I280	K214	A152	K89	T28
D470	G409	G409	A347	G215	D153	H90	K29
A471	D410	D410	S348	K216	L154	N91	Y30
T472	S411	S411	Y349		Y155	V82	S31
K473	K412	K412	R350	H219	E156	E93	Y32
F474	V413	V413	H351	L220	A157	F94	E33
	A414	A414	L352	L221	M158	Q95	V36
F477	M415	M415	G353	K222	Q159	T96	V37
Y478	D416	D416	N354	I223	R160	K97	T38
P479	E417	E417	N355	R224	S161	E98	T39
V480	Y418	Y418	D356	R225	Q162	G99	K39
L481	Y419	Y419	G357	D226	V163	V100	T40
			Y358	I227	L164	K101	A41
F483	L422	L422	N359	Q228	E165	Q102	S42
L484	M423	M423	L360	N229	Y166	P103	G43
S485	L424	L424	S361	P297	D167	N104	R44
Y486	G495	G495	A362	K231	L168	Y105	F45
W487	G426	G426	F363	E232	F106	F106	D46
L488	H427	H427	K364	E233	G107	G107	V47
K489	N428	N428	Q365	F301	R170	S108	T48
A490	R429	R429	F366	V302	L172	M109	P49
P491	I430	I430	R367	P303	K173	T110	T50
	S431	S431	S368	Q304	A174	Q111	V51
T493	I432	I432	K369	L305	K175		Q52
R494	H433	H433	E370	V306	M176	T114	D53
P496	V435	V435	I371	Q307	S177	L115	Y54
G496	M434	M434	S372	L308	L178	K116	V55
F497	C436	C436	K373	A309	V179		F56
H498	E437	E437	S374	E310		I119	K57
P499	D438	D438	S375	H311		D120	L58
V500	S439	S439	V376	N246	P183	A121	D59
N501	L440	L440	I377	T247	S184	E122	L60
G502	L441	L441	D378	F315	I185	G123	K61

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, α , β , γ	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 ²)	42.0	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: NH4, DG6, NAI

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	2.38	189/4219 (4.5%)	1.95	155/5719 (2.7%)
1	B	2.51	231/4211 (5.5%)	2.11	193/5708 (3.4%)
All	All	2.44	420/8430 (5.0%)	2.03	348/11427 (3.0%)

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	5
1	B	0	7
All	All	0	12

The worst 5 of 420 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	423	MET	SD-CE	-15.93	1.39	1.79
1	B	158	MET	SD-CE	15.00	2.17	1.79
1	B	71	ILE	CA-CB	-14.56	1.36	1.54
1	A	459	VAL	CA-CB	13.88	1.72	1.54
1	A	69	MET	SD-CE	13.73	2.13	1.79

The worst 5 of 348 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	526	LEU	CA-C-N	-16.70	100.15	123.20
1	B	526	LEU	C-N-CA	-16.70	100.15	123.20
1	B	318	GLY	N-CA-C	15.96	130.81	110.38
1	B	325	GLN	N-CA-C	-14.71	93.59	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	SER	N-CA-C	-13.03	90.69	110.10

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	450	1
1	B	4130	0	4136	529	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	9	0
4	B	44	0	24	2	0
5	A	303	0	0	57	0
5	B	315	0	0	64	0
All	All	9006	0	8353	941	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 56.

The worst 5 of 941 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:CG	1:B:69:MET:CB	1.82	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:MET:CG	1:A:136:MET:SD	2.02	1.46
1:B:69:MET:SD	1:B:69:MET:CE	2.08	1.40
1:A:415:MET:SD	1:A:415:MET:CE	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 [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	523/533 (98%)	463 (88%)	37 (7%)	23 (4%)	2	1
1	B	522/533 (98%)	444 (85%)	52 (10%)	26 (5%)	1	0
All	All	1045/1066 (98%)	907 (87%)	89 (8%)	49 (5%)	2	0

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%)	389 (84%)	75 (16%)	2	2
1	B	463/471 (98%)	377 (81%)	86 (19%)	1	1
All	All	927/942 (98%)	766 (83%)	161 (17%)	2	2

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	273	GLU
1	B	457	THR
1	B	315	PHE
1	B	364	LYS
1	B	492	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	ASN
1	B	428	ASN
1	B	91	ASN
1	B	398	HIS
1	B	523	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	DG6	B	640	-	14,14,14	4.05	9 (64%)	18,19,19	2.25	5 (27%)
3	DG6	A	630	-	14,14,14	4.76	10 (71%)	18,19,19	2.53	7 (38%)
4	NAI	A	650	-	47,48,48	3.86	32 (68%)	64,73,73	2.27	18 (28%)
4	NAI	B	660	-	47,48,48	3.76	30 (63%)	64,73,73	2.31	26 (40%)

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	DG6	B	640	-	1/1/4/4	8/17/17/17	-
3	DG6	A	630	-	1/1/4/4	10/17/17/17	-
4	NAI	A	650	-	-	7/29/72/72	0/5/5/5
4	NAI	B	660	-	-	2/29/72/72	0/5/5/5

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	630	DG6	C6-C5	9.76	1.65	1.51
3	B	640	DG6	C6-C5	9.27	1.64	1.51
4	B	660	NAI	PA-O3	8.93	1.69	1.59
4	B	660	NAI	C4A-N3A	8.64	1.50	1.34
4	A	650	NAI	PA-O3	7.95	1.68	1.59

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	650	NAI	O4D-C1D-N1N	7.82	123.00	108.08
4	A	650	NAI	O2A-PA-O1A	6.28	141.64	112.44
4	B	660	NAI	O4D-C1D-N1N	5.63	118.82	108.08
3	A	630	DG6	C6-C5-C4	5.58	122.75	112.22
4	A	650	NAI	O7N-C7N-N7N	-5.55	110.45	122.89

All (2) chirality outliers are listed below:

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

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	630	DG6	C2-C3-C4-C5
3	A	630	DG6	O4-C4-C5-O5
3	A	630	DG6	O5-C5-C6-O6
3	B	640	DG6	O1-C1-C2-C3
3	B	640	DG6	C2-C3-C4-O4

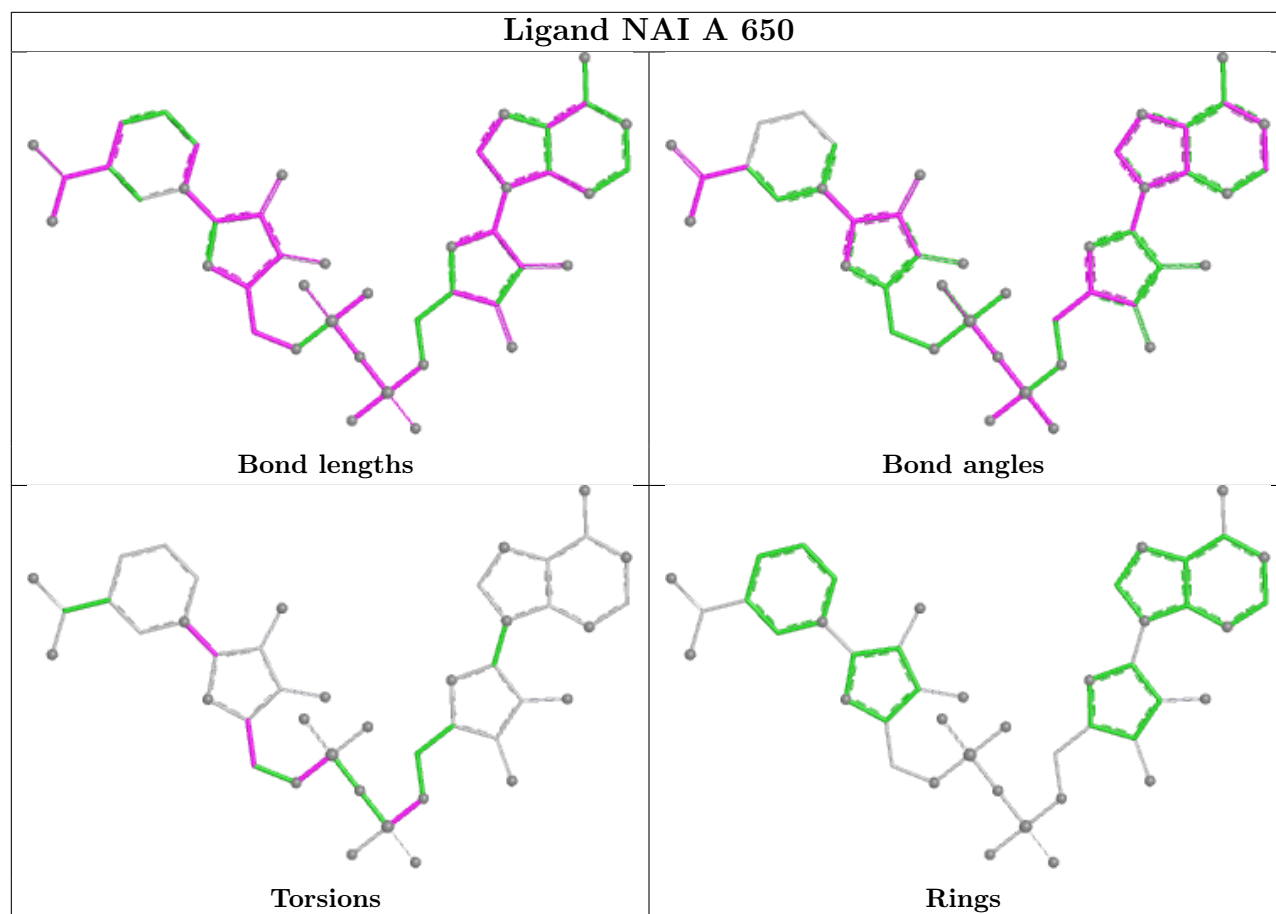
There are no ring outliers.

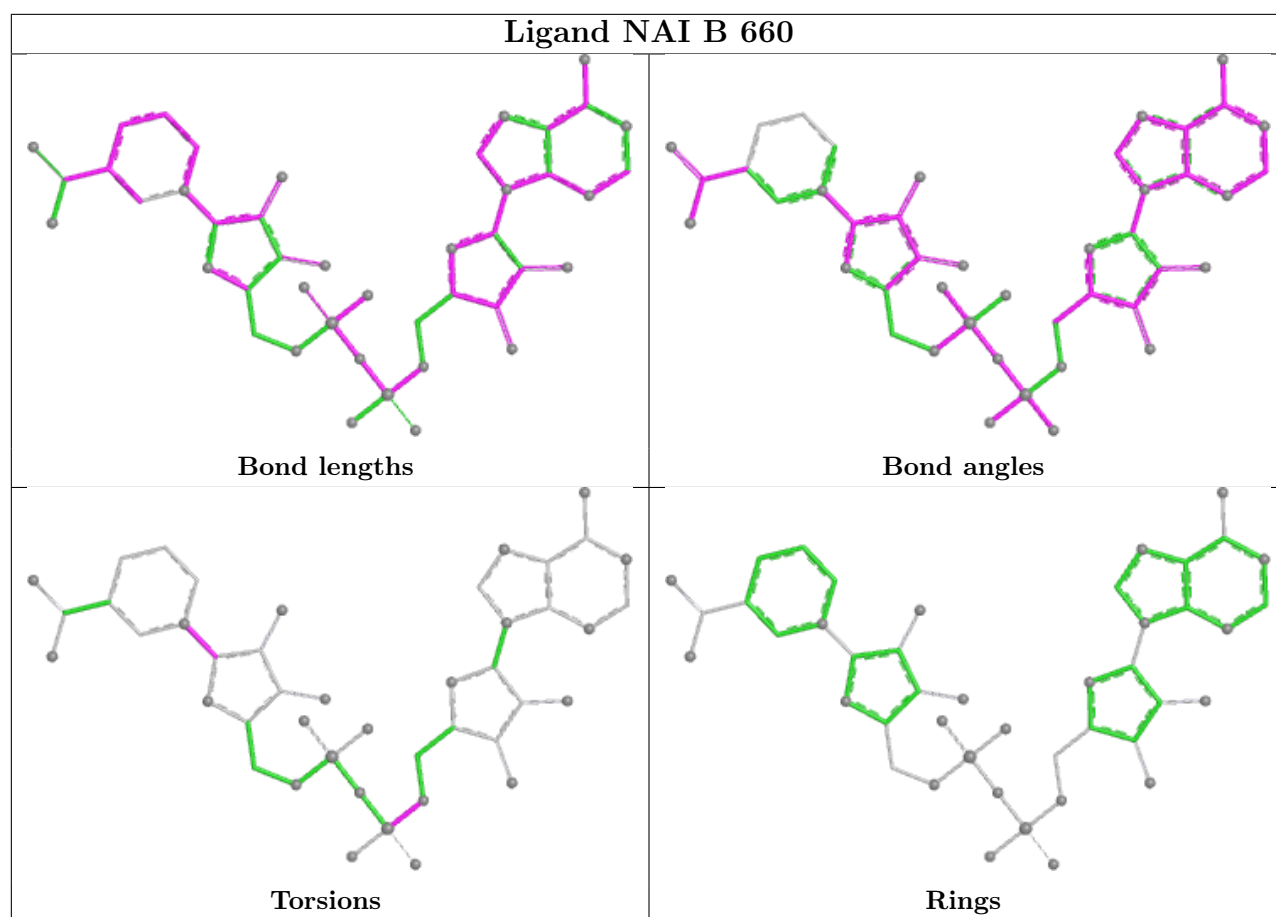
4 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	640	DG6	17	0
3	A	630	DG6	10	0
4	A	650	NAI	9	0
4	B	660	NAI	2	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.