wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:16 PM GMT

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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

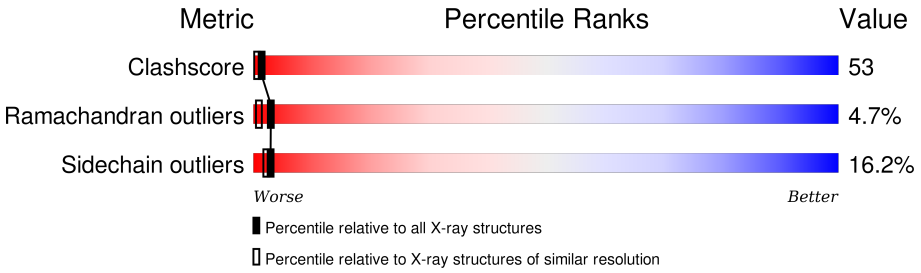
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (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 >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	533	34% 43% 17% 5%
1	B	533	28% 41% 23% 7%

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	-
3	DG6	B	640	X	-	X	-

2 Entry composition (i)

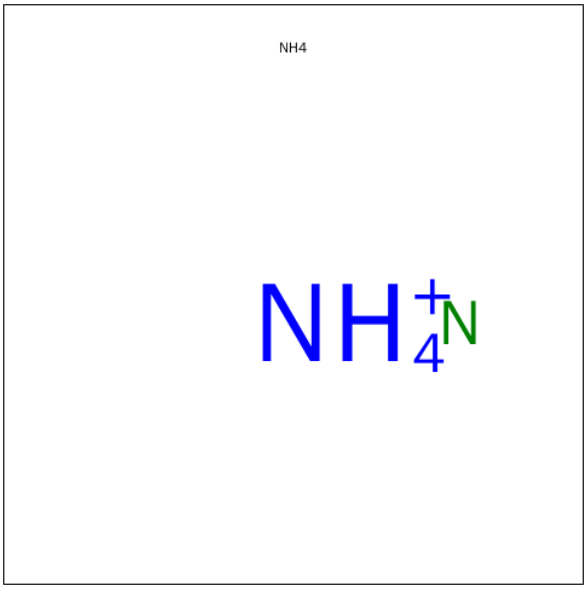
There are 5 unique types of molecules in this entry. The entry contains 9006 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

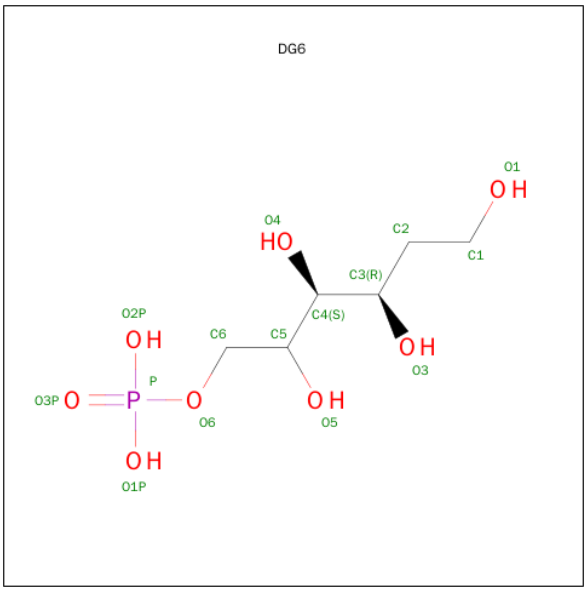
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4138	2632	695	795	16			
1	B	524	Total	C	N	O	S	0	0	0
			4130	2626	694	794	16			

- Molecule 2 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



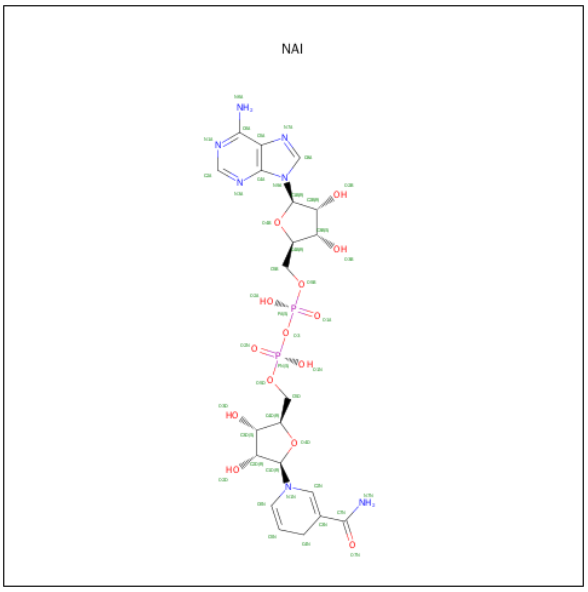
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N	0	0
			1	1		
2	B	1	Total	N	0	0
			1	1		

- Molecule 3 is 2-DEOXY-GLUCITOL-6-PHOSPHATE (three-letter code: DG6) (formula: $C_6H_{15}O_8P$).



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: $C_{21}H_{29}N_7O_{14}P_2$).



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		

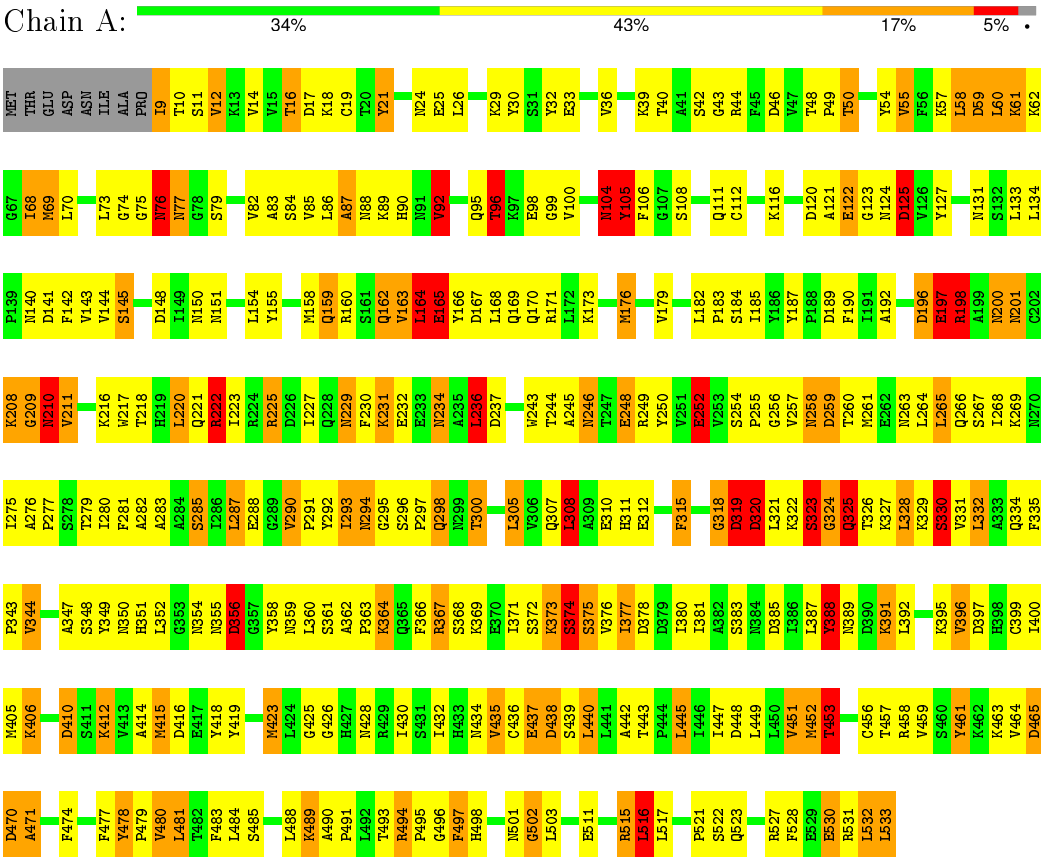
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

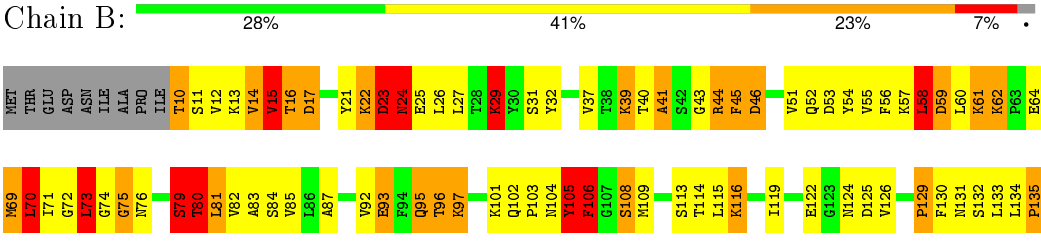
- Molecule 1: myo-inositol-1-phosphate synthase

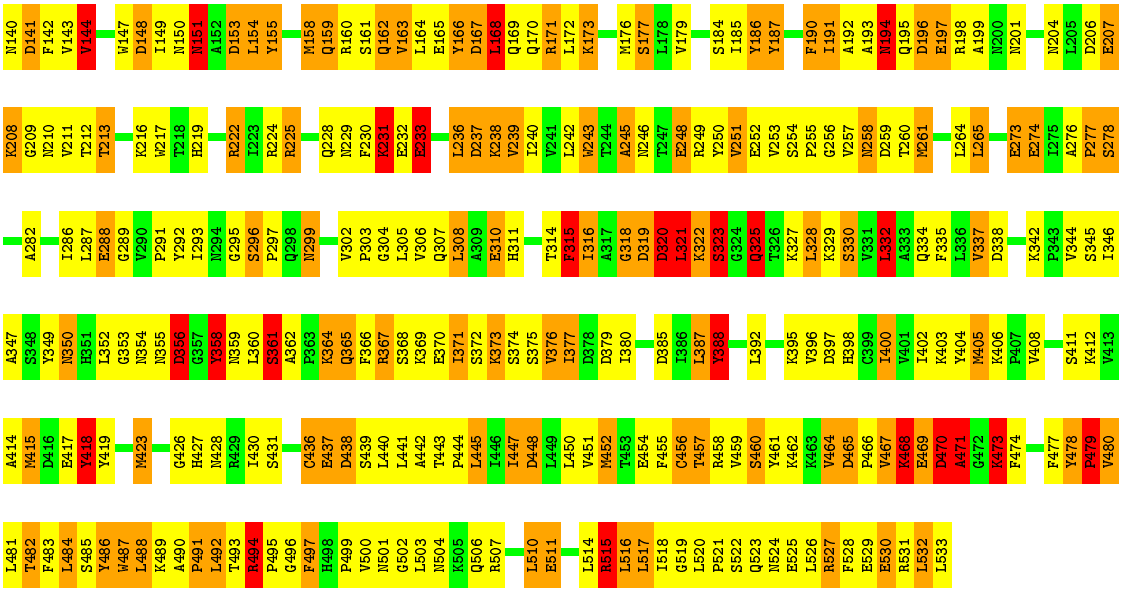
Chain A:



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

Chain B:




N140 D141 F142 V143 V144 W147 D148 I149 N150 N151 A152 D153 L154 Y155 M158 Q159 R160 S161 Q162 V163 L164 E165 Y166 D167 L168 Q169 Q170 R171 L172 K173 M176 S177 L178 V179 S184 I185 Y186 Y187 F190 I191 A192 A193 N194 Q195 D196 E197 R198 A199 N200 N201 N204 L205 D206 E207
K208 G209 N210 V211 T212 T213 K216 W217 T218 H219 R222 I223 R224 R225 Q228 N229 F230 K231 E232 E233 L236 D237 K238 V239 I240 V241 L242 W243 T244 A245 N246 T247 E248 R249 Y250 V251 E252 V253 S254 P255 G256 V257 N258 D259 T260 M261 L264 L265 E273 E274 I275 A276 P277 S278
A282 I286 L287 E288 G289 V290 P291 Y292 I293 N294 G295 S296 P297 Q298 N299 V302 P303 G304 L305 V306 Q307 L308 A309 E310 H311 T314 F315 I316 A317 G318 D319 D320 L321 K322 S323 G324 Q325 T326 K327 L328 K329 S330 V331 L332 A333 Q334 F335 L336 V337 D338 K342 P343 V344 S345 I346
A347 S348 Y349 N350 H351 L352 G353 N354 N355 D356 G357 K358 N359 L360 S361 A362 P363 K364 Q365 F366 R367 S368 K369 E370 I371 S372 K373 S374 S375 V376 I377 D378 D379 I380 D385 I386 I387 Y388 I392 K395 V396 D397 H398 C399 I400 V401 I402 K403 Y404 M405 K406 P407 V408 S411 K412 V413
A414 M415 D416 E417 V418 Y419 M423 G426 H427 N428 R429 I430 S431 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 S485 Y486 W487 L488 K489 A490 P491 L492 T493 R494 P495 G496 F497 H498 P499 V500 N501 G502 L503 N504 K505 Q506 R507 L510 E511 L514 R515 L516 L517 I518 G519 L520 P521 S522 Q523 N524 E525 L526 R527 F528 E529 E530 R531 L532 L533

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 1.0	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, 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (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	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 (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%)	3	1
1	B	522/533 (98%)	444 (85%)	52 (10%)	26 (5%)	3	1
All	All	1045/1066 (98%)	907 (87%)	89 (8%)	49 (5%)	3	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%)	4 3
1	B	463/471 (98%)	381 (82%)	82 (18%)	2 1
All	All	927/942 (98%)	777 (84%)	150 (16%)	3 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 (i)

There are no carbohydrates 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	A	630	-	14,14,14	4.33	10 (71%)	15,19,19	1.72	3 (20%)
4	NAI	A	650	-	38,48,48	3.45	23 (60%)	48,73,73	2.19	12 (25%)
3	DG6	B	640	-	14,14,14	3.66	9 (64%)	15,19,19	1.75	3 (20%)
4	NAI	B	660	-	38,48,48	3.83	20 (52%)	48,73,73	2.61	22 (45%)

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

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	660	NAI	O4B-C1B	-12.85	1.25	1.41
4	A	650	NAI	O2B-C2B	-8.21	1.23	1.43
4	A	650	NAI	O4B-C1B	-7.33	1.31	1.41
4	B	660	NAI	O2B-C2B	-5.74	1.29	1.43
4	A	650	NAI	PA-O1A	-5.40	1.31	1.51

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	660	NAI	C1B-N9A-C4A	-5.73	118.30	126.94
4	A	650	NAI	O7N-C7N-N7N	-4.95	110.45	122.76
4	A	650	NAI	C1B-N9A-C4A	-4.93	119.51	126.94
4	B	660	NAI	O2D-C2D-C1D	-4.20	95.27	109.94
4	B	660	NAI	C4B-O4B-C1B	-3.97	105.36	109.72

All (2) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 36 short contacts:

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

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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.