



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:24 PM UTC

PDB ID : 2ACQ / pdb_00002acq
Title : AN ANION BINDING SITE IN HUMAN ALDOSE REDUCTASE: MECHANISTIC IMPLICATIONS FOR THE BINDING OF CITRATE, CACODYLATE, AND GLUCOSE-6-PHOSPHATE
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Deposited on : 1994-04-15
Resolution : 1.76 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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)
Xtrriage (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

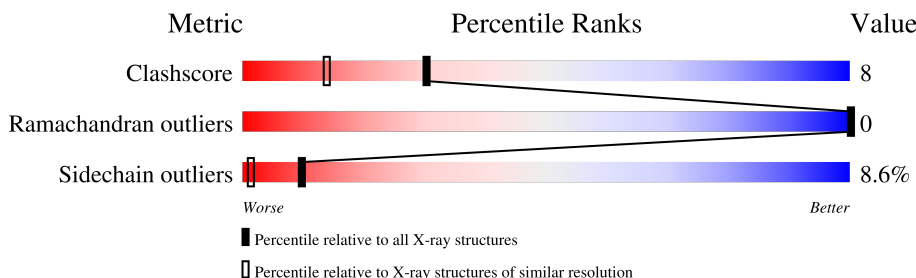
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)

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	315	80% 17% .

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	G6P	A	317	X	-	-	-

2 Entry composition [i](#)

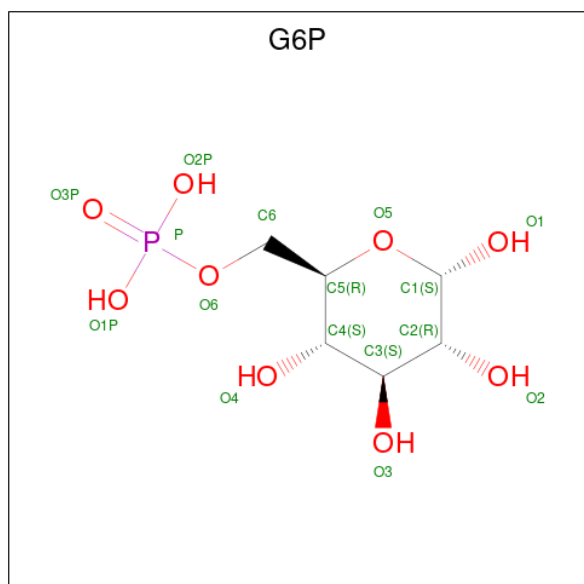
There are 4 unique types of molecules in this entry. The entry contains 2763 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALDOSE REDUCTASE.

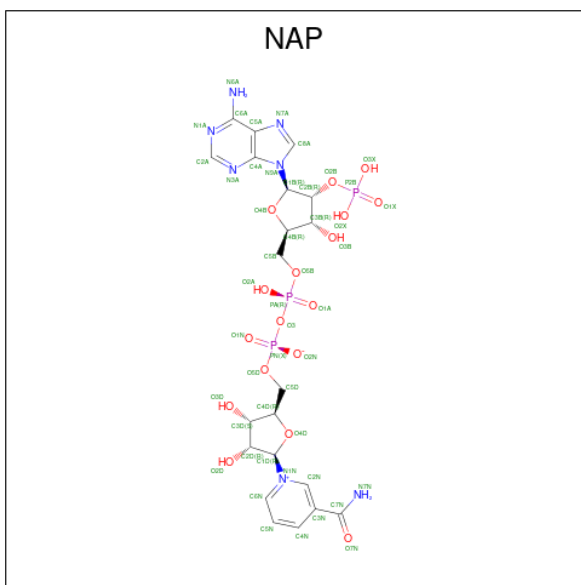
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	315	2517	1617	425	463	12	0	0	0

- Molecule 2 is 6-O-phosphono-alpha-D-glucopyranose (CCD ID: G6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	16	6	9	1	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is water.

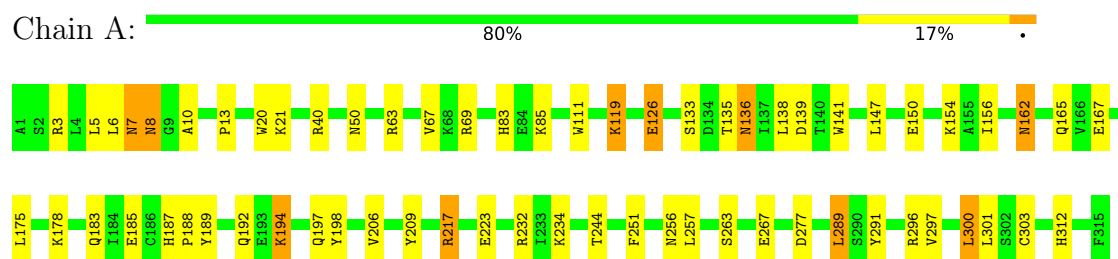
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	182	Total O 182 182	0	0

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: ALDOSE REDUCTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.94Å 67.17Å 91.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.76	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.76)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2763	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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: NAP, G6P

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	0.66	0/2579	0.81	0/3502

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	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	TYR	Sidechain
1	A	296	ARG	Sidechain
1	A	40	ARG	Sidechain
1	A	69	ARG	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	2517	0	2533	43	0
2	A	16	0	11	1	0
3	A	48	0	25	3	0
4	A	182	0	0	8	0
All	All	2763	0	2569	43	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 8.

All (43) 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:A:83:HIS:HD2	4:A:469:HOH:O	1.69	0.75
1:A:217:ARG:HD3	1:A:297:VAL:HG13	1.75	0.67
1:A:162:ASN:C	1:A:162:ASN:HD22	2.03	0.67
1:A:251:PHE:HZ	1:A:289:LEU:HD13	1.66	0.60
1:A:7:ASN:ND2	4:A:482:HOH:O	2.35	0.60
1:A:183:GLN:NE2	3:A:316:NAP:H2N	2.17	0.59
1:A:8:ASN:HD22	1:A:8:ASN:H	1.51	0.59
1:A:256:ASN:HA	4:A:481:HOH:O	2.04	0.57
1:A:194:LYS:H	1:A:194:LYS:HZ2	1.51	0.56
1:A:183:GLN:NE2	3:A:316:NAP:H71N	2.04	0.55
1:A:185:GLU:OE2	1:A:187:HIS:HE1	1.92	0.52
1:A:136:ASN:HD22	1:A:138:LEU:H	1.57	0.51
1:A:167:GLU:HG2	1:A:198:TYR:OH	2.12	0.50
1:A:277:ASP:HB3	4:A:475:HOH:O	2.11	0.50
1:A:300:LEU:HD13	1:A:303:CYS:HB2	1.94	0.49
1:A:187:HIS:HD2	1:A:189:TYR:H	1.61	0.49
1:A:83:HIS:HE1	4:A:455:HOH:O	1.97	0.48
1:A:111:TRP:HE1	2:A:317:G6P:H62	1.79	0.48
1:A:119:LYS:H	1:A:119:LYS:NZ	2.13	0.47
1:A:8:ASN:HD22	1:A:8:ASN:N	2.12	0.46
1:A:162:ASN:C	1:A:162:ASN:ND2	2.71	0.46
1:A:251:PHE:CZ	1:A:289:LEU:HD13	2.49	0.46
1:A:20:TRP:CE3	1:A:21:LYS:HE3	2.51	0.46
1:A:232:ARG:HB3	1:A:291:TYR:OH	2.16	0.46
1:A:20:TRP:O	1:A:21:LYS:HB2	2.15	0.46
1:A:234:LYS:HG2	1:A:244:THR:HG21	1.99	0.44
1:A:136:ASN:HD22	1:A:138:LEU:N	2.16	0.44
1:A:154:LYS:HE2	1:A:154:LYS:HB3	1.82	0.43
1:A:126:GLU:H	1:A:126:GLU:HG3	1.71	0.43
1:A:141:TRP:CZ2	1:A:156:ILE:HD12	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:VAL:HB	1:A:257:LEU:HD22	2.00	0.43
1:A:187:HIS:HB2	1:A:188:PRO:HD2	2.01	0.42
1:A:6:LEU:HB2	1:A:8:ASN:ND2	2.35	0.42
1:A:136:ASN:ND2	1:A:139:ASP:H	2.18	0.42
1:A:133:SER:OG	1:A:135:THR:HG23	2.21	0.41
1:A:8:ASN:ND2	1:A:10:ALA:H	2.18	0.41
1:A:83:HIS:CD2	4:A:469:HOH:O	2.56	0.41
1:A:312:HIS:CE1	4:A:400:HOH:O	2.73	0.41
1:A:312:HIS:HE1	4:A:400:HOH:O	2.03	0.41
1:A:234:LYS:HA	1:A:244:THR:HG22	2.02	0.41
1:A:3:ARG:HG2	1:A:13:PRO:HA	2.04	0.40
1:A:162:ASN:ND2	1:A:165:GLN:H	2.19	0.40
1:A:263:SER:HA	3:A:316:NAP:O1X	2.21	0.40

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	313/315 (99%)	309 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	280/280 (100%)	256 (91%)	24 (9%)	10 1

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	7	ASN
1	A	8	ASN
1	A	50	ASN
1	A	63	ARG
1	A	67	VAL
1	A	85	LYS
1	A	119	LYS
1	A	126	GLU
1	A	136	ASN
1	A	147	LEU
1	A	150	GLU
1	A	162	ASN
1	A	175	LEU
1	A	178	LYS
1	A	192	GLN
1	A	194	LYS
1	A	197	GLN
1	A	217	ARG
1	A	223	GLU
1	A	267	GLU
1	A	289	LEU
1	A	300	LEU
1	A	301	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	8	ASN
1	A	26	GLN
1	A	50	ASN
1	A	52	ASN
1	A	59	GLN
1	A	83	HIS
1	A	93	GLN
1	A	110	HIS

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Mol	Chain	Res	Type
1	A	136	ASN
1	A	160	ASN
1	A	162	ASN
1	A	183	GLN
1	A	187	HIS
1	A	200	GLN
1	A	283	GLN
1	A	312	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](#)

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	G6P	A	317	-	16,16,16	2.73	8 (50%)	23,24,24	2.18	12 (52%)
3	NAP	A	316	-	50,52,52	1.43	9 (18%)	71,80,80	1.76	18 (25%)

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	G6P	A	317	-	1/1/6/6	6/6/26/26	0/1/1/1
3	NAP	A	316	-	-	2/35/67/67	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	G6P	C4-C5	6.23	1.66	1.53
3	A	316	NAP	C2N-N1N	4.32	1.39	1.35
2	A	317	G6P	C6-C5	4.22	1.64	1.51
2	A	317	G6P	C3-C2	3.80	1.62	1.52
3	A	316	NAP	C3N-C7N	3.63	1.56	1.50
3	A	316	NAP	C6N-N1N	3.54	1.43	1.35
2	A	317	G6P	C1-C2	3.10	1.59	1.52
2	A	317	G6P	C4-C3	2.99	1.60	1.52
3	A	316	NAP	O4D-C1D	2.91	1.44	1.40
2	A	317	G6P	P-O3P	2.65	1.58	1.50
3	A	316	NAP	C4A-N9A	-2.51	1.32	1.37
3	A	316	NAP	PA-O2A	-2.46	1.44	1.55
2	A	317	G6P	O3-C3	2.38	1.48	1.43
3	A	316	NAP	PN-O3	2.30	1.62	1.59
3	A	316	NAP	P2B-O3X	-2.26	1.46	1.54
3	A	316	NAP	C5A-N7A	-2.20	1.35	1.39
2	A	317	G6P	P-O2P	2.02	1.62	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	316	NAP	N3A-C4A-N9A	4.83	135.39	127.17
3	A	316	NAP	C5A-C4A-N3A	-4.78	120.13	126.72
2	A	317	G6P	O2-C2-C3	4.11	120.08	110.38
3	A	316	NAP	N3A-C2A-N1A	-3.87	122.72	128.58
2	A	317	G6P	C3-C4-C5	3.85	117.21	110.23
2	A	317	G6P	O5-C5-C4	3.62	116.22	109.70
3	A	316	NAP	C4A-N9A-C8A	3.52	109.44	105.74
3	A	316	NAP	C6N-N1N-C2N	-3.49	118.91	121.88
3	A	316	NAP	C6A-C5A-C4A	3.46	121.90	117.18
2	A	317	G6P	O6-C6-C5	3.28	120.15	108.99
3	A	316	NAP	C6A-C5A-N7A	-3.22	125.88	132.09
2	A	317	G6P	C1-O5-C5	3.18	119.80	113.65
3	A	316	NAP	O2A-PA-O3	2.81	114.86	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	G6P	C6-C5-C4	2.73	117.80	112.07
3	A	316	NAP	N9A-C8A-N7A	-2.67	110.16	113.94
3	A	316	NAP	C6N-C5N-C4N	-2.60	115.71	119.45
2	A	317	G6P	O6-P-O3P	-2.58	99.47	106.44
3	A	316	NAP	C2A-N3A-C4A	2.57	118.10	111.83
2	A	317	G6P	O2P-P-O1P	2.39	116.77	107.80
3	A	316	NAP	C5N-C4N-C3N	2.22	122.55	120.36
3	A	316	NAP	O2D-C2D-C3D	-2.21	104.72	111.82
2	A	317	G6P	O4-C4-C3	-2.20	105.19	110.38
3	A	316	NAP	C5N-C6N-N1N	2.17	123.34	120.38
2	A	317	G6P	O5-C5-C6	2.17	111.00	106.69
3	A	316	NAP	O4B-C4B-C3B	2.17	109.45	105.15
3	A	316	NAP	C4A-N9A-C1B	-2.16	121.58	126.63
2	A	317	G6P	O1-C1-C2	2.16	115.24	108.98
3	A	316	NAP	O4D-C4D-C3D	-2.15	100.89	105.15
2	A	317	G6P	O4-C4-C5	2.08	114.45	109.32
3	A	316	NAP	C2A-N1A-C6A	2.06	122.12	118.73

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	317	G6P	C1

All (8) torsion outliers are listed below:

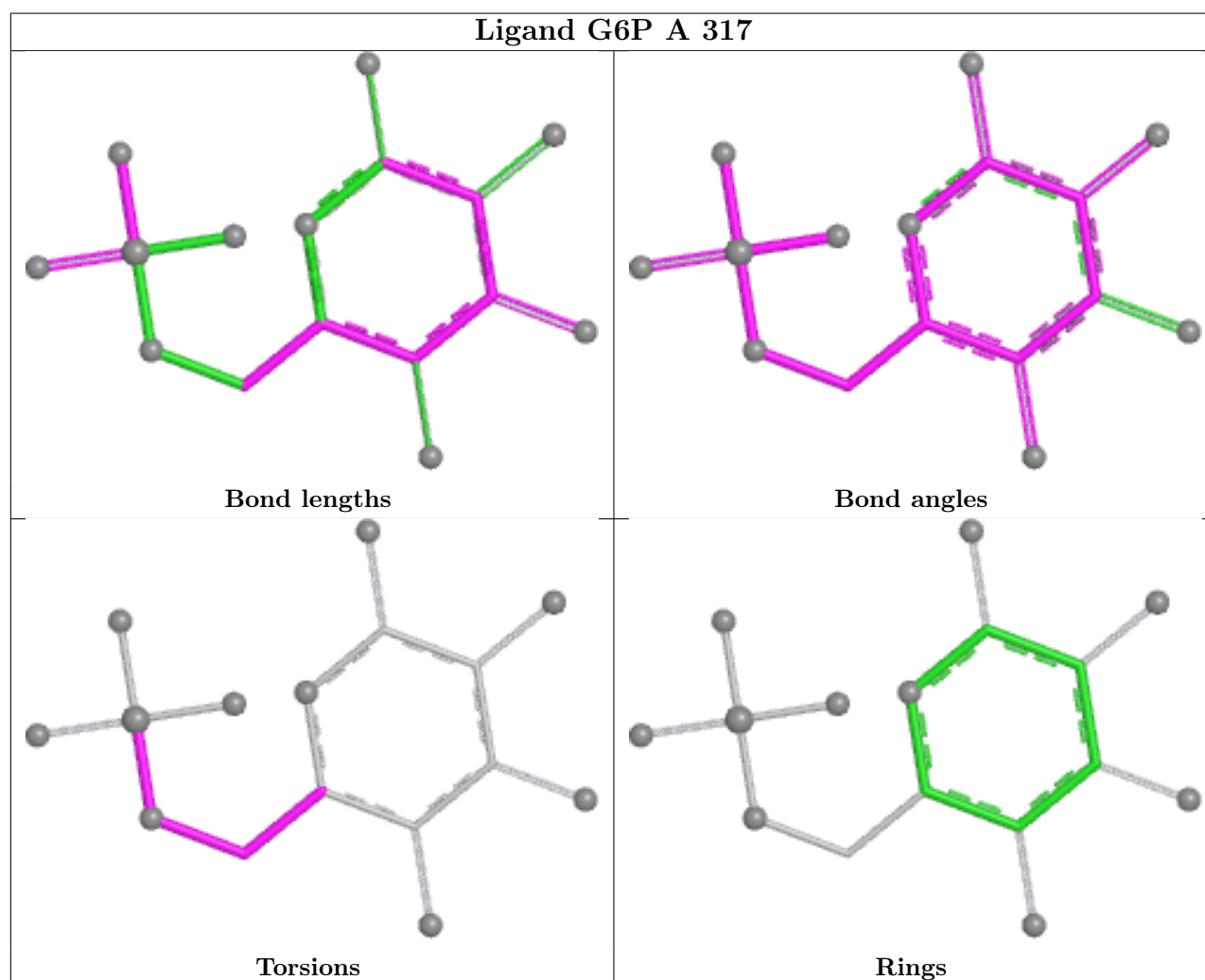
Mol	Chain	Res	Type	Atoms
2	A	317	G6P	C4-C5-C6-O6
2	A	317	G6P	O5-C5-C6-O6
2	A	317	G6P	C6-O6-P-O1P
2	A	317	G6P	C6-O6-P-O2P
2	A	317	G6P	C6-O6-P-O3P
2	A	317	G6P	C5-C6-O6-P
3	A	316	NAP	PA-O3-PN-O5D
3	A	316	NAP	C4D-C5D-O5D-PN

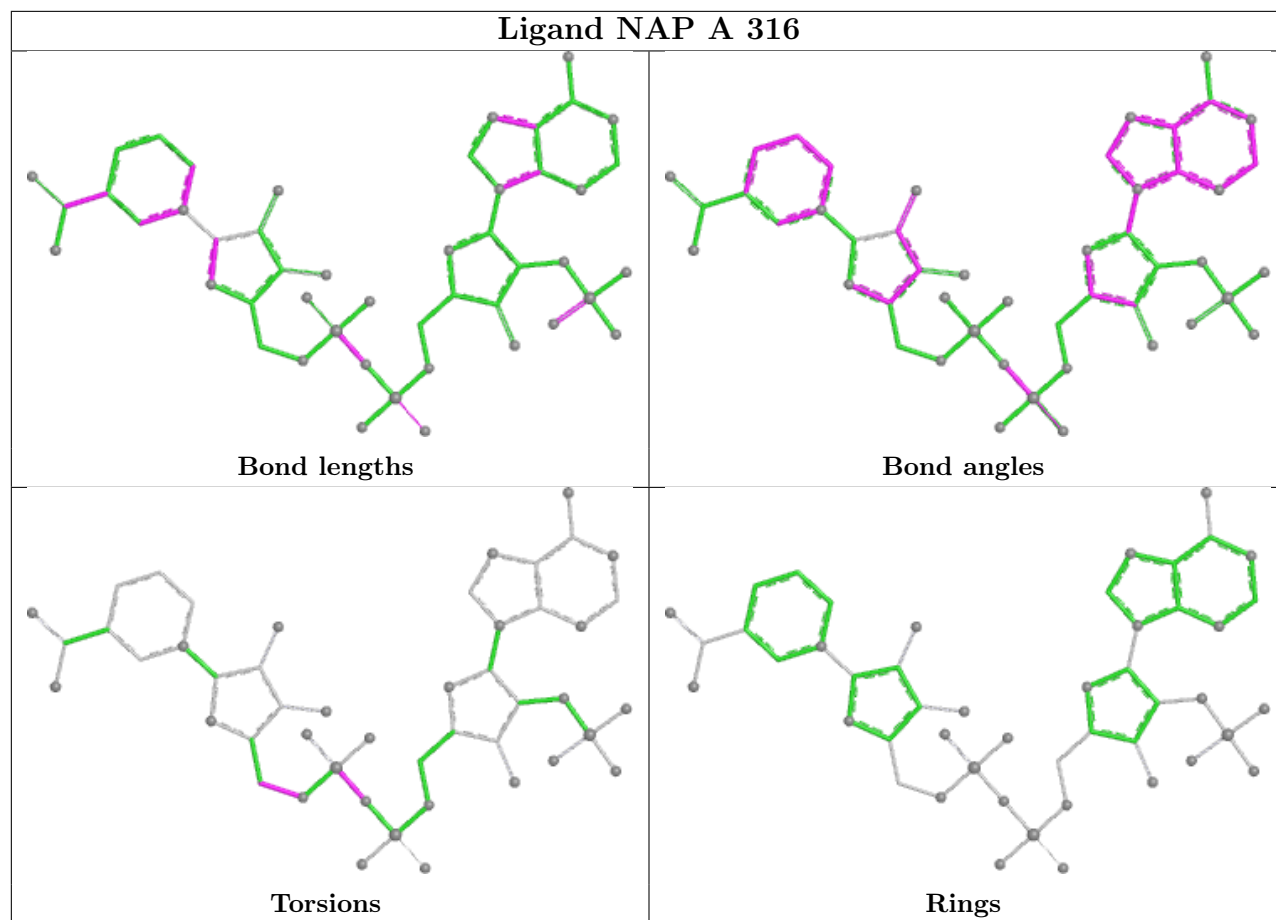
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	317	G6P	1	0
3	A	316	NAP	3	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.