



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 03:46 AM EST

PDB ID : 1EQU
Title : TYPE 1 17-BETA HYDROXYSTEROID DEHYDROGENASE EQUILIN
COMPLEXED WITH NADP+
Authors : Sawicki, M.W.; Erman, M.; Puranen, T.; Vihko, P.; Ghosh, D.
Deposited on : 1998-12-02
Resolution : 3.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

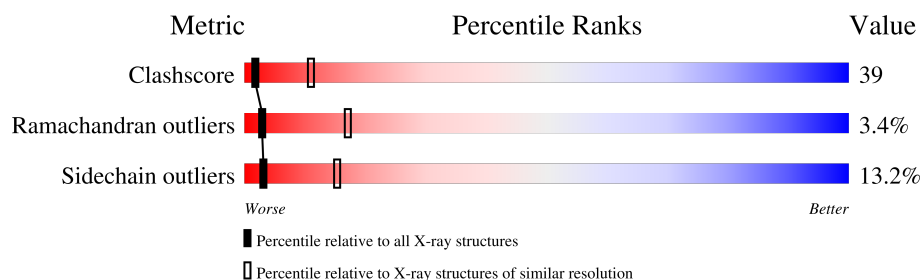
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)

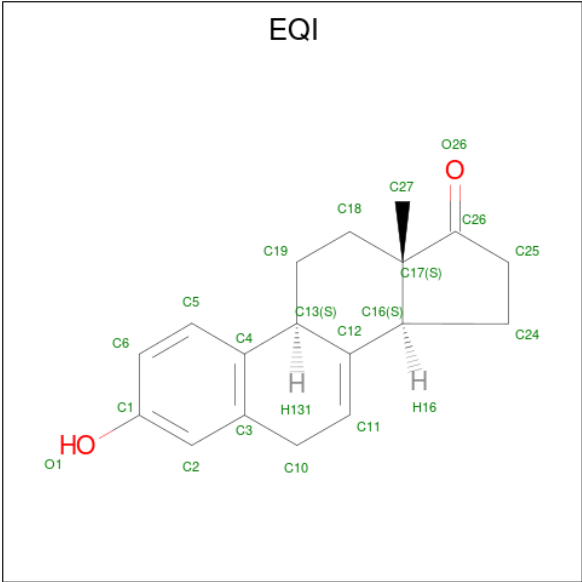
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	327	
1	B	327	

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	NAP	A	328	X	-	X	-
2	NAP	B	328	X	-	X	-
3	EQU	A	329	-	-	X	-



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C	O	0
			20	18	2	

- Molecule 4 is water.

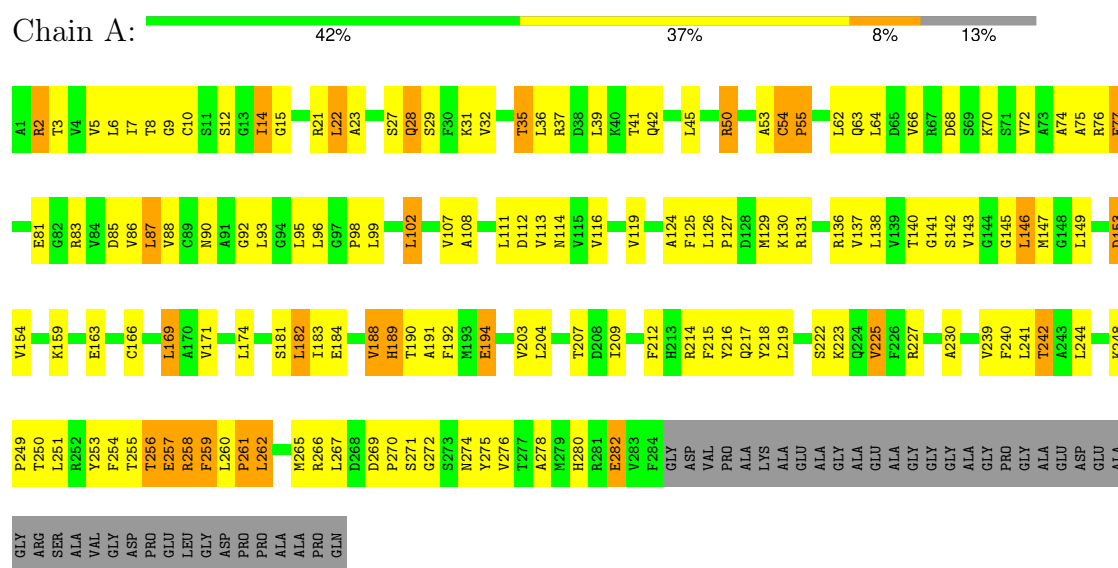
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	O	0	0
			12	12		
4	B	6	Total	O	0	0
			6	6		

3 Residue-property plots

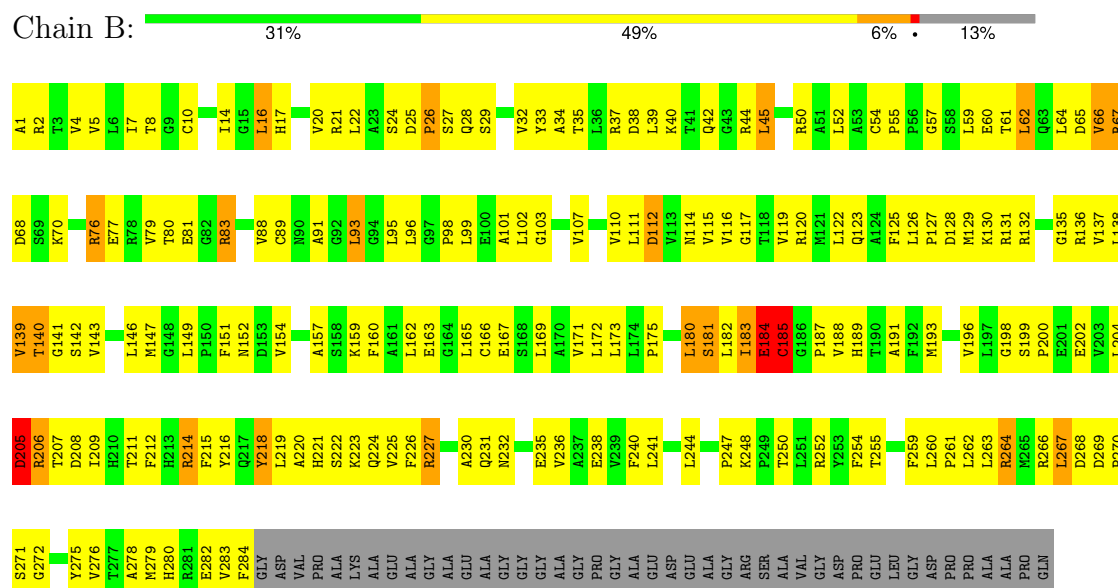
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: PROTEIN (ESTRADIOL 17 BETA-DEHYDROGENASE 1)



• Molecule 1: PROTEIN (ESTRADIOL 17 BETA-DEHYDROGENASE 1)



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	44.02Å 114.16Å 114.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.00	Depositor
% Data completeness (in resolution range)	93.1 (12.00-3.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.182 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4488	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: EQI, NAP

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	0.55	0/2218	0.75	0/3009
1	B	0.56	1/2218 (0.0%)	0.82	5/3009 (0.2%)
All	All	0.55	1/4436 (0.0%)	0.78	5/6018 (0.1%)

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	B	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	ASP	C-N	11.62	1.60	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	CYS	CA-C-N	-10.14	95.92	116.20
1	B	205	ASP	O-C-N	-8.97	108.34	122.70
1	B	185	CYS	O-C-N	7.79	136.44	123.20
1	B	62	LEU	CA-CB-CG	6.36	129.92	115.30
1	B	185	CYS	C-N-CA	-6.34	108.98	122.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	185	CYS	Mainchain
1	B	205	ASP	Mainchain
1	B	218	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	2177	0	2218	160	2
1	B	2177	0	2218	197	2
2	A	48	0	21	28	0
2	B	48	0	21	23	0
3	A	20	0	19	12	0
4	A	12	0	0	0	0
4	B	6	0	0	0	0
All	All	4488	0	4497	352	2

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 39.

The worst 5 of 352 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:199:SER:CB	1:B:216:TYR:HE2	1.44	1.29
1:B:199:SER:CB	1:B:216:TYR:CE2	2.17	1.28
1:B:199:SER:HB3	1:B:216:TYR:CE2	1.69	1.27
1:B:204:LEU:HD13	1:B:212:PHE:CE1	1.68	1.27
1:B:188:VAL:CA	1:B:231:GLN:O	1.92	1.16

All (2) 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:216:TYR:CE1	1:B:198:GLY:O[3_655]	1.65	0.55
1:A:216:TYR:CD1	1:B:198:GLY:O[3_655]	1.96	0.24

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	282/327 (86%)	249 (88%)	25 (9%)	8 (3%)	4	21
1	B	282/327 (86%)	237 (84%)	34 (12%)	11 (4%)	2	14
All	All	564/654 (86%)	486 (86%)	59 (10%)	19 (3%)	3	17

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	55	PRO
1	B	28	GLN
1	B	66	VAL
1	B	184	GLU

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	235/257 (91%)	205 (87%)	30 (13%)	3	16
1	B	235/257 (91%)	203 (86%)	32 (14%)	3	14
All	All	470/514 (91%)	408 (87%)	62 (13%)	3	15

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	ASN

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Mol	Chain	Res	Type
1	B	185	CYS
1	B	45	LEU
1	B	184	GLU
1	B	248	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	28	GLN
1	B	123	GLN
1	B	280	HIS
1	A	213	HIS
1	A	231	GLN

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](#)

3 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	NAP	A	328	-	46,52,52	2.49	9 (19%)	61,80,80	3.78	25 (40%)
2	NAP	B	328	-	46,52,52	2.46	13 (28%)	61,80,80	4.74	37 (60%)
3	EQI	A	329	-	23,23,23	1.74	4 (17%)	24,36,36	1.18	2 (8%)

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	NAP	A	328	-	5/5/12/12	10/31/67/67	0/5/5/5
2	NAP	B	328	-	6/6/12/12	12/31/67/67	0/5/5/5
3	EQI	A	329	-	-	-	0/4/4/4

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	328	NAP	C2N-N1N	9.40	1.45	1.35
2	A	328	NAP	C2N-N1N	9.15	1.45	1.35
2	A	328	NAP	PA-O3	-7.41	1.51	1.59
2	A	328	NAP	O4D-C1D	6.37	1.49	1.40
2	B	328	NAP	O4B-C1B	6.14	1.49	1.40

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	328	NAP	C3N-C7N-N7N	-21.13	91.71	117.74
2	A	328	NAP	C3N-C7N-N7N	-17.12	96.64	117.74
2	B	328	NAP	O7N-C7N-N7N	10.77	138.17	122.62
2	A	328	NAP	O7N-C7N-N7N	10.66	138.01	122.62
2	A	328	NAP	C2B-C1B-N9A	9.83	134.38	112.56

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	328	NAP	C3D
2	A	328	NAP	C4B
2	A	328	NAP	C3B
2	A	328	NAP	C2B
2	A	328	NAP	C2D

5 of 22 torsion outliers are listed below:

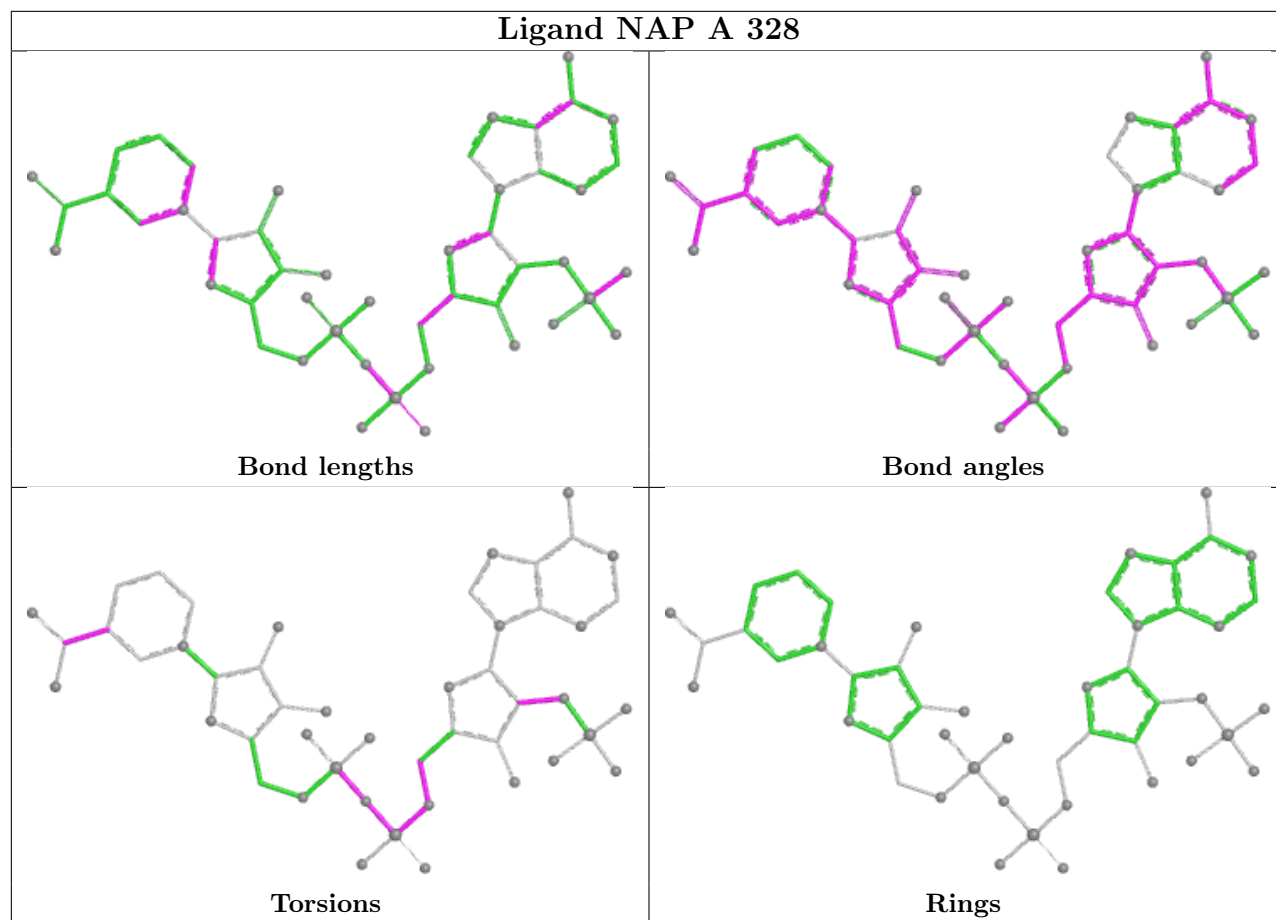
Mol	Chain	Res	Type	Atoms
2	A	328	NAP	C5B-O5B-PA-O1A
2	A	328	NAP	C5B-O5B-PA-O3
2	A	328	NAP	C4B-C5B-O5B-PA
2	A	328	NAP	PA-O3-PN-O5D
2	B	328	NAP	C5B-O5B-PA-O1A

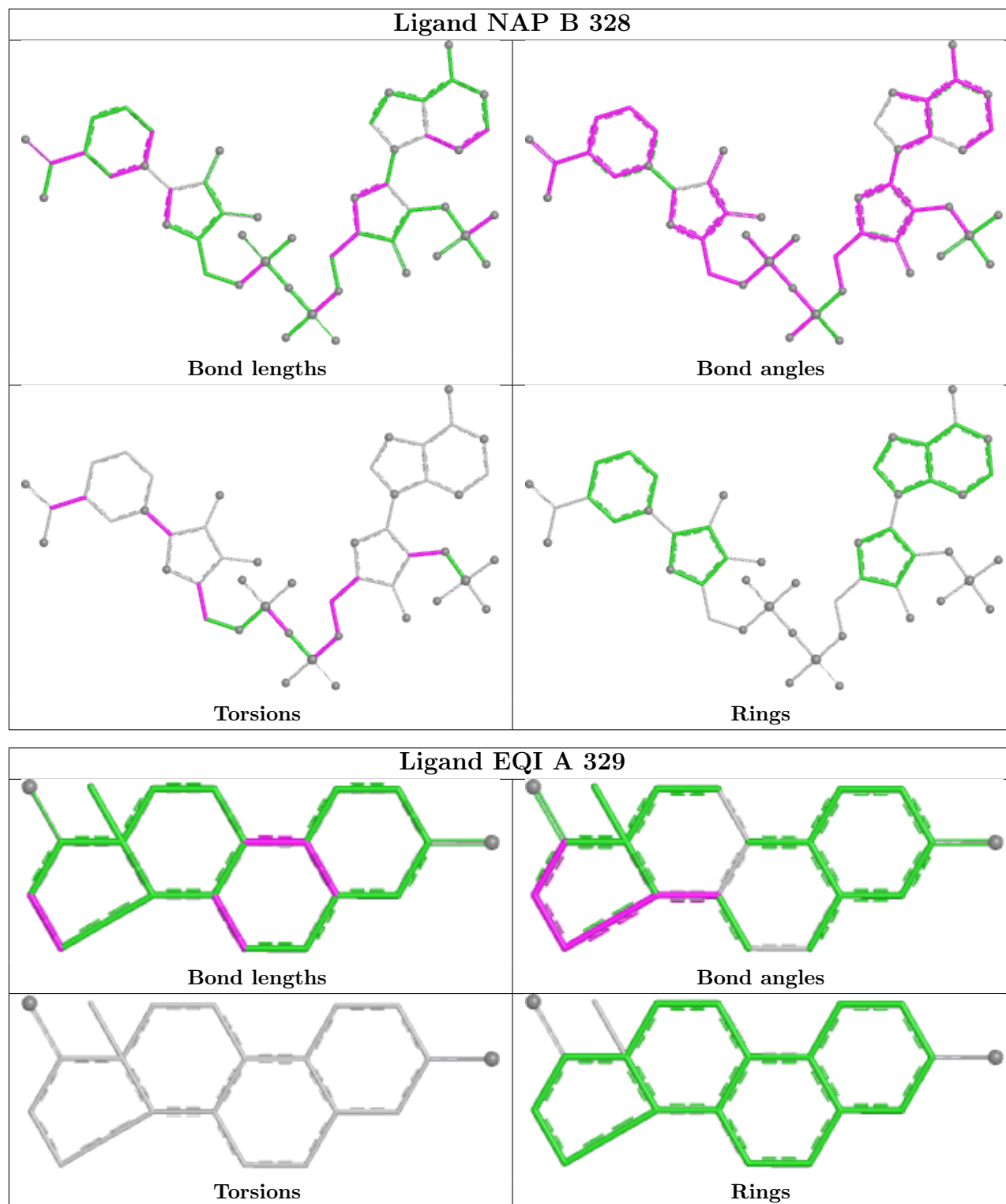
There are no ring outliers.

3 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	328	NAP	28	0
2	B	328	NAP	23	0
3	A	329	EQI	12	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	205:ASP	C	206:ARG	N	1.60

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.