WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2024 – 06:36 PM EST

PDB ID	:	1QI1
Title	:	Ternary Complex of an NADP Dependent Aldehyde Dehydrogenase
Authors	:	Cobessi, D.; Tete-Favier, F.; Marchal, S.; Branlant, G.; Aubry, A.
Deposited on	:	1999-06-02
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:

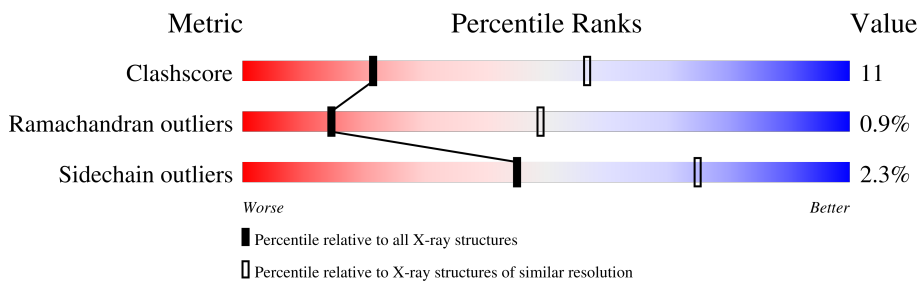|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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	Percentile Ranks	Value
Clashscore		11
Ramachandran outliers		0.9%
Sidechain outliers		2.3%

Worse — Better

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	475	76% 23% •
1	B	475	78% 21% •
1	C	475	78% 21% •
1	D	475	79% 20% •

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	B	501	-	-	X	-
3	G3H	A	504	-	-	X	-
3	G3H	C	506	-	-	X	-
3	G3H	D	507	-	-	X	-
4	G3P	B	505	X	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 14616 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 PROTEIN (NADP-DEPENDENT NONPHOSPHORYLAT-ING GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE).

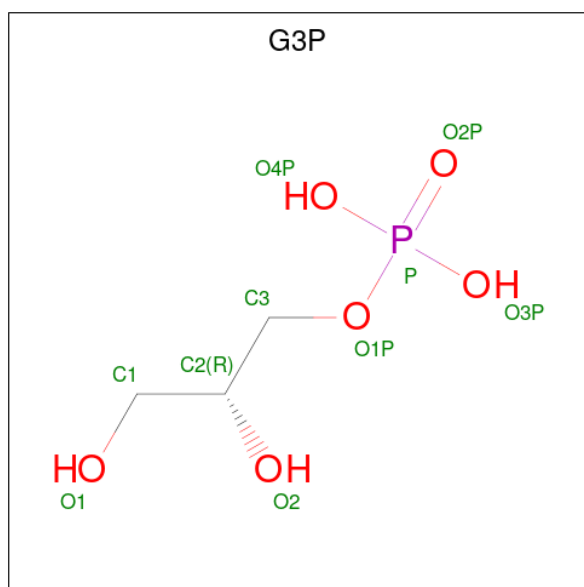| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3596	2286	600	700	10			
1	B	474	Total	C	N	O	S	0	0	0
			3596	2286	600	700	10			
1	C	474	Total	C	N	O	S	0	0	0
			3596	2286	600	700	10			
1	D	474	Total	C	N	O	S	0	0	0
			3596	2286	600	700	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	SER	CYS	engineered mutation	UNP Q59931
B	284	SER	CYS	engineered mutation	UNP Q59931
C	284	SER	CYS	engineered mutation	UNP Q59931
D	284	SER	CYS	engineered mutation	UNP Q59931

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

NAP

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

- Molecule 3 is GLYCERALDEHYDE-3-PHOSPHATE (three-letter code: G3H) (formula: $C_3H_7O_6P$).

G3H

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	D	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 4 is SN-GLYCEROL-3-PHOSPHATE (three-letter code: G3P) (formula: $C_3H_9O_6P$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			10	3	6	1		

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.
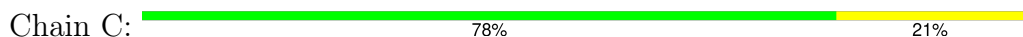
Note EDS was not executed.

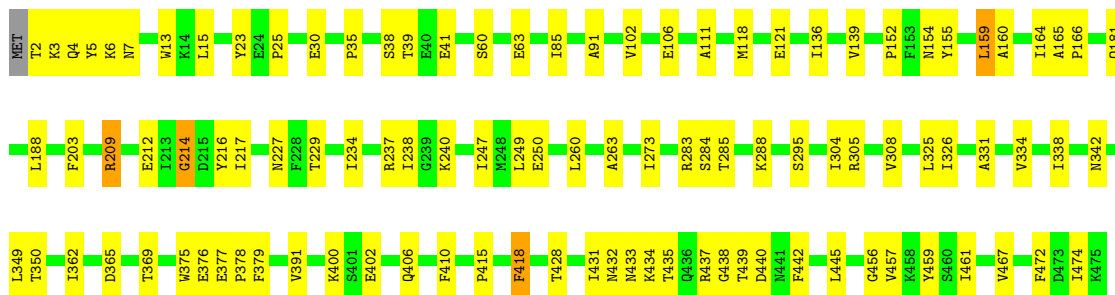• Molecule 1: PROTEIN (NADP-DEPENDENT NONPHOSPHORYLATING GLYCERALDEH YDE-3-PHOSPHATE DEHYDROGENASE)
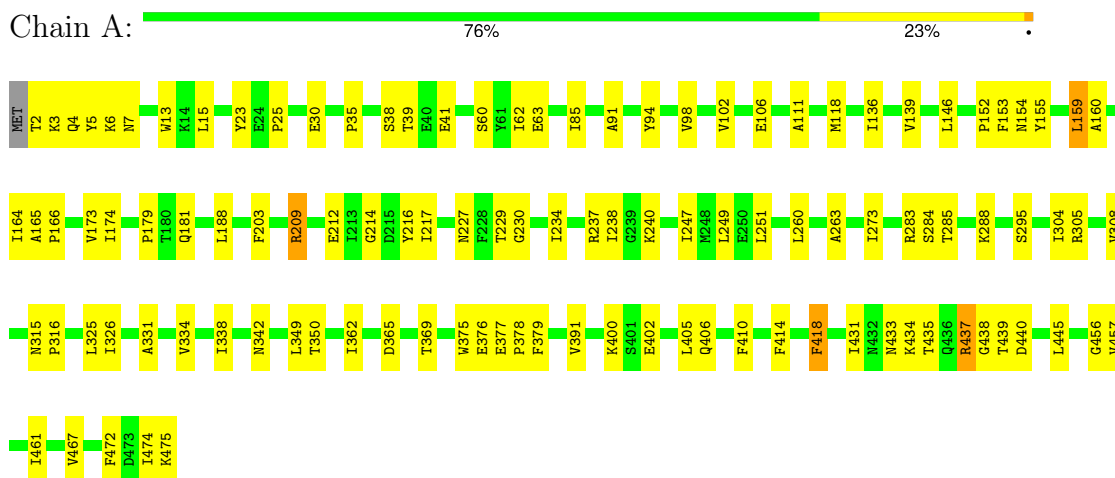
• Molecule 1: PROTEIN (NADP-DEPENDENT NONPHOSPHORYLATING GLYCERALDEH YDE-3-PHOSPHATE DEHYDROGENASE)
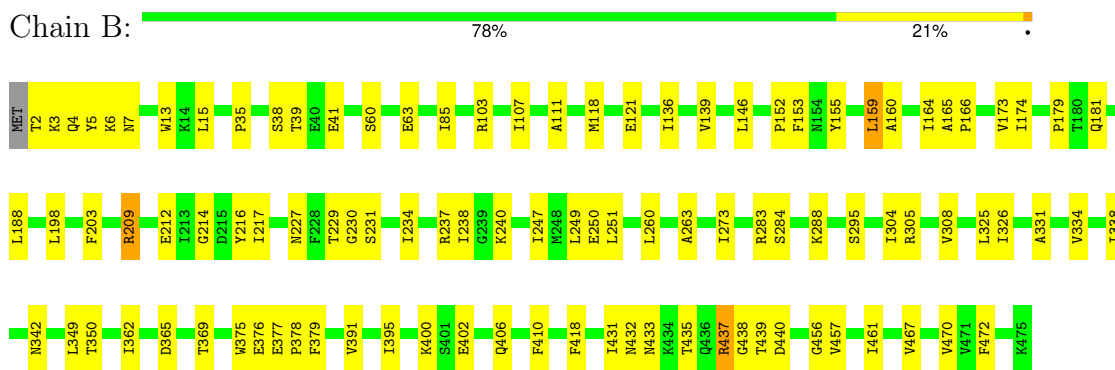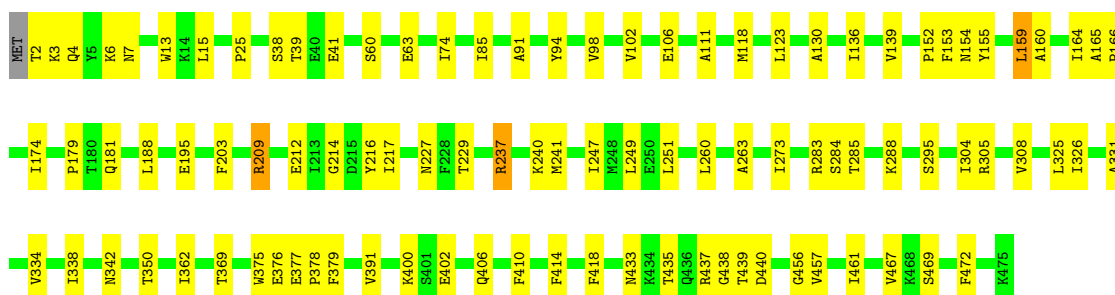

• Molecule 1: PROTEIN (NADP-DEPENDENT NONPHOSPHORYLATING GLYCERALDEH YDE-3-PHOSPHATE DEHYDROGENASE)

• Molecule 1: PROTEIN (NADP-DEPENDENT NONPHOSPHORYLATING GLYCERALDEH YDE-3-PHOSPHATE DEHYDROGENASE)

Chain D:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.50Å 158.50Å 282.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	75.0 (8.00-3.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.242 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14616	wwPDB-VP
Average B, all atoms (Å^2)	14.0	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, G3H, G3P

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	0.50	0/3654	0.82	11/4942 (0.2%)
1	B	0.52	0/3654	0.72	11/4942 (0.2%)
1	C	0.50	0/3654	0.89	13/4942 (0.3%)
1	D	0.52	0/3654	0.90	13/4942 (0.3%)
All	All	0.51	0/14616	0.84	48/19768 (0.2%)

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	209	ARG	NE-CZ-NH2	-21.16	109.72	120.30
1	A	209	ARG	NE-CZ-NH1	20.22	130.41	120.30
1	C	283	ARG	NE-CZ-NH1	19.87	130.23	120.30
1	D	305	ARG	NE-CZ-NH2	-19.61	110.49	120.30
1	D	437	ARG	NE-CZ-NH1	19.03	129.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3596	0	3649	89	0
1	B	3596	0	3649	70	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3596	0	3649	82	0
1	D	3596	0	3649	71	0
2	A	48	0	25	16	0
2	B	48	0	25	21	0
2	C	48	0	25	19	0
2	D	48	0	25	13	0
3	A	10	0	5	9	0
3	C	10	0	5	8	0
3	D	10	0	5	8	0
4	B	10	0	6	11	0
All	All	14616	0	14717	313	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 11.

The worst 5 of 313 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:D:284:SER:HB3	2:D:503:NAP:C4N	1.60	1.31
1:C:285:THR:OG1	3:C:506:G3H:H31	1.41	1.18
1:C:284:SER:HB3	2:C:502:NAP:C5N	1.78	1.14
1:D:284:SER:HB3	2:D:503:NAP:C5N	1.79	1.12
1:D:284:SER:CB	2:D:503:NAP:C4N	2.28	1.10

There are no symmetry-related clashes.

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	472/475 (99%)	444 (94%)	24 (5%)	4 (1%)	16	51
1	B	472/475 (99%)	443 (94%)	25 (5%)	4 (1%)	16	51

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	472/475 (99%)	443 (94%)	24 (5%)	5 (1%)	12	44
1	D	472/475 (99%)	445 (94%)	23 (5%)	4 (1%)	16	51
All	All	1888/1900 (99%)	1775 (94%)	96 (5%)	17 (1%)	14	49

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	THR
1	B	439	THR
1	C	439	THR
1	D	439	THR
1	A	438	GLY

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	378/379 (100%)	369 (98%)	9 (2%)	44	74
1	B	378/379 (100%)	369 (98%)	9 (2%)	44	74
1	C	378/379 (100%)	370 (98%)	8 (2%)	48	77
1	D	378/379 (100%)	369 (98%)	9 (2%)	44	74
All	All	1512/1516 (100%)	1477 (98%)	35 (2%)	45	75

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	174	ILE
1	D	227	ASN
1	D	369	THR
1	B	227	ASN
1	B	174	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	227	ASN
1	D	342	ASN
1	C	342	ASN
1	D	412	ASN
1	C	433	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	#$|Z| > 2$
3	G3H	D	507	-	8,9,9	1.41	2 (25%)	7,12,12	0.89	0
4	G3P	B	505	-	9,9,9	1.45	1 (11%)	10,12,12	0.96	0
2	NAP	C	502	-	46,52,52	2.84	7 (15%)	61,80,80	2.59	17 (27%)
3	G3H	A	504	-	8,9,9	1.37	1 (12%)	7,12,12	0.96	0
2	NAP	B	501	-	46,52,52	2.12	6 (13%)	61,80,80	3.14	20 (32%)
2	NAP	A	500	-	46,52,52	2.31	6 (13%)	61,80,80	2.85	16 (26%)
3	G3H	C	506	-	8,9,9	1.57	3 (37%)	7,12,12	0.93	0
2	NAP	D	503	-	46,52,52	2.35	9 (19%)	61,80,80	2.03	15 (24%)

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	G3H	D	507	-	-	5/7/8/8	-
4	G3P	B	505	-	1/1/2/2	0/8/8/8	-
2	NAP	C	502	-	-	11/31/67/67	0/5/5/5
3	G3H	A	504	-	-	3/7/8/8	-
2	NAP	B	501	-	-	8/31/67/67	0/5/5/5
2	NAP	A	500	-	-	12/31/67/67	0/5/5/5
3	G3H	C	506	-	-	3/7/8/8	-
2	NAP	D	503	-	-	7/31/67/67	0/5/5/5

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	502	NAP	C3N-C7N	-15.61	1.27	1.50
2	B	501	NAP	C3N-C7N	-10.94	1.34	1.50
2	A	500	NAP	C3N-C7N	-10.85	1.34	1.50
2	D	503	NAP	C3N-C7N	-10.74	1.34	1.50
2	A	500	NAP	PA-O3	-6.21	1.52	1.59

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAP	C4D-O4D-C1D	-18.97	92.55	109.92
2	A	500	NAP	C4D-O4D-C1D	-17.07	94.29	109.92
2	C	502	NAP	C4D-O4D-C1D	-14.90	96.28	109.92
2	D	503	NAP	C4D-O4D-C1D	-9.07	101.62	109.92
2	C	502	NAP	P2B-O2B-C2B	-6.90	105.01	123.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	505	G3P	C2

5 of 49 torsion outliers are listed below:

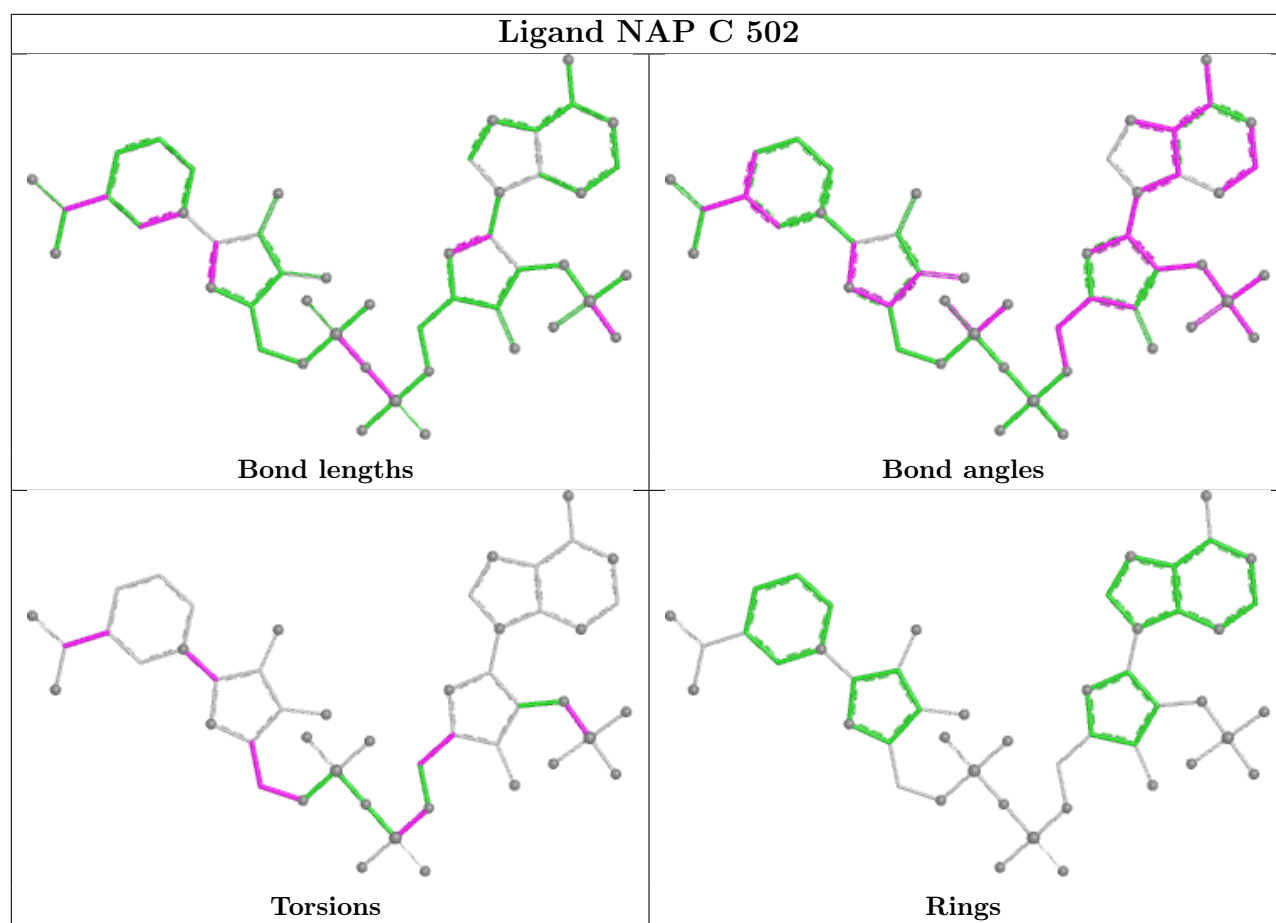| Mol	Chain	Res	Type	Atoms
2	A	500	NAP	C5B-O5B-PA-O1A

Continued on next page...

Continued from previous page...

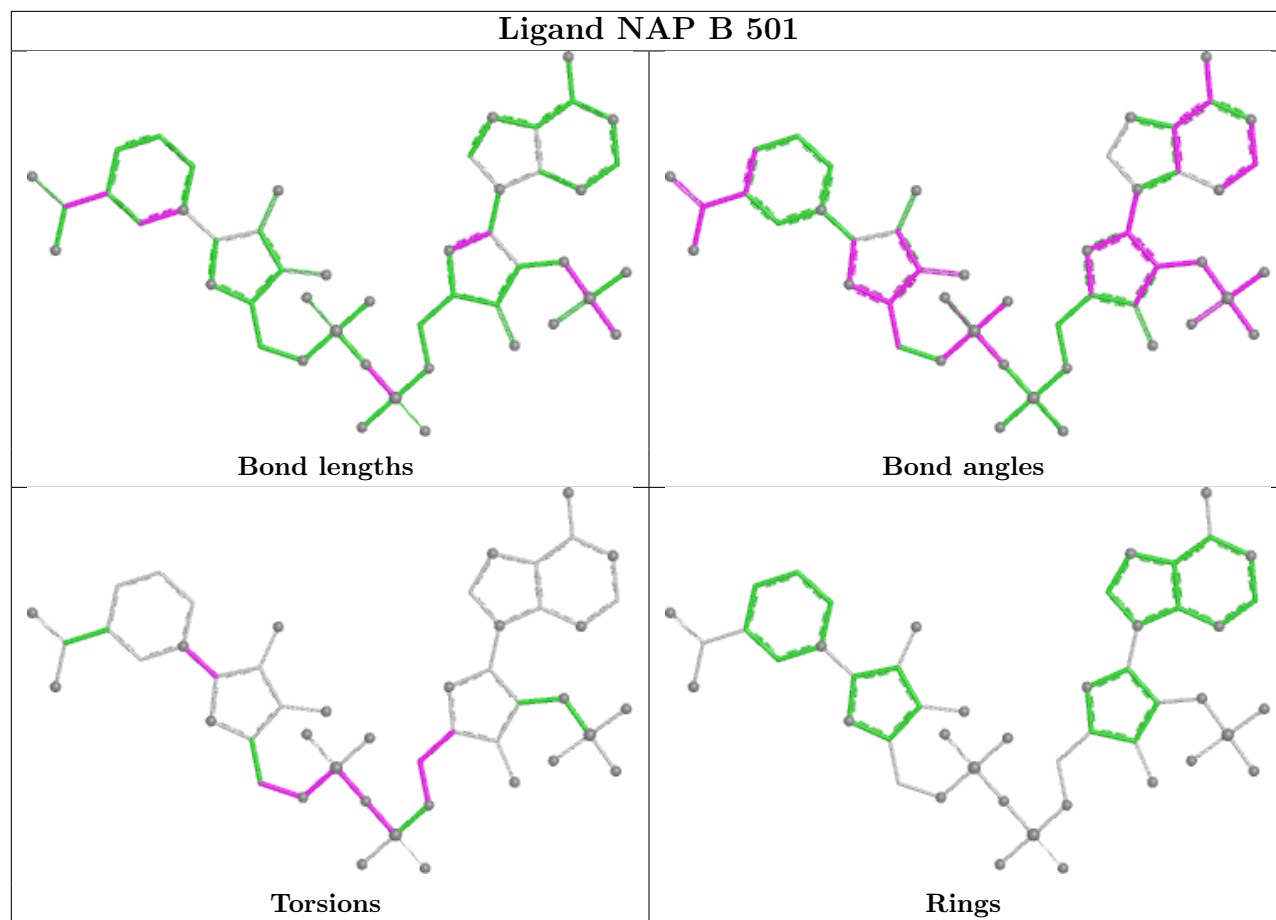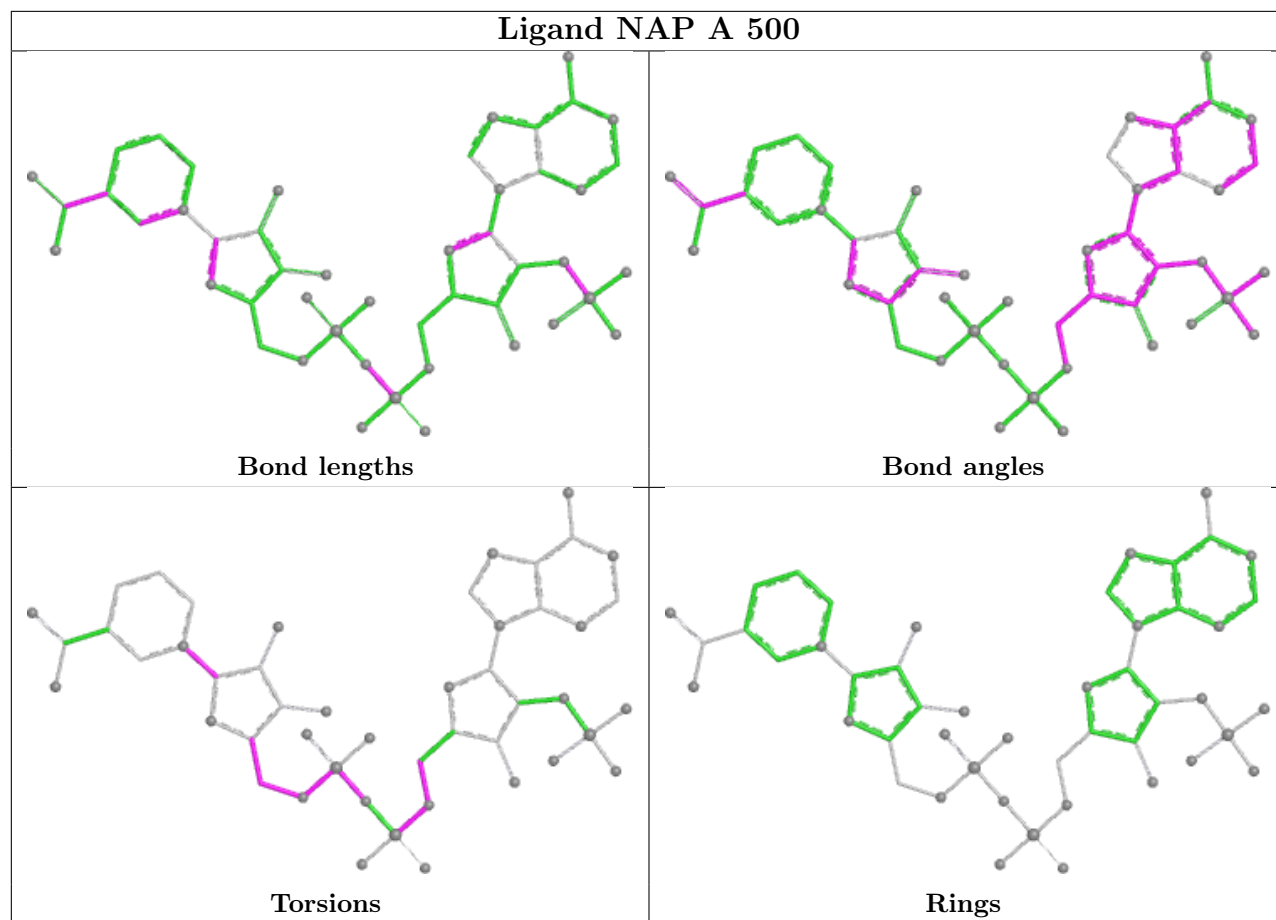| Mol	Chain	Res	Type	Atoms
2	A	500	NAP	C5B-O5B-PA-O2A
2	A	500	NAP	C5B-O5B-PA-O3
2	A	500	NAP	C5D-O5D-PN-O2N
2	A	500	NAP	C2D-C1D-N1N-C2N

There are no ring outliers.
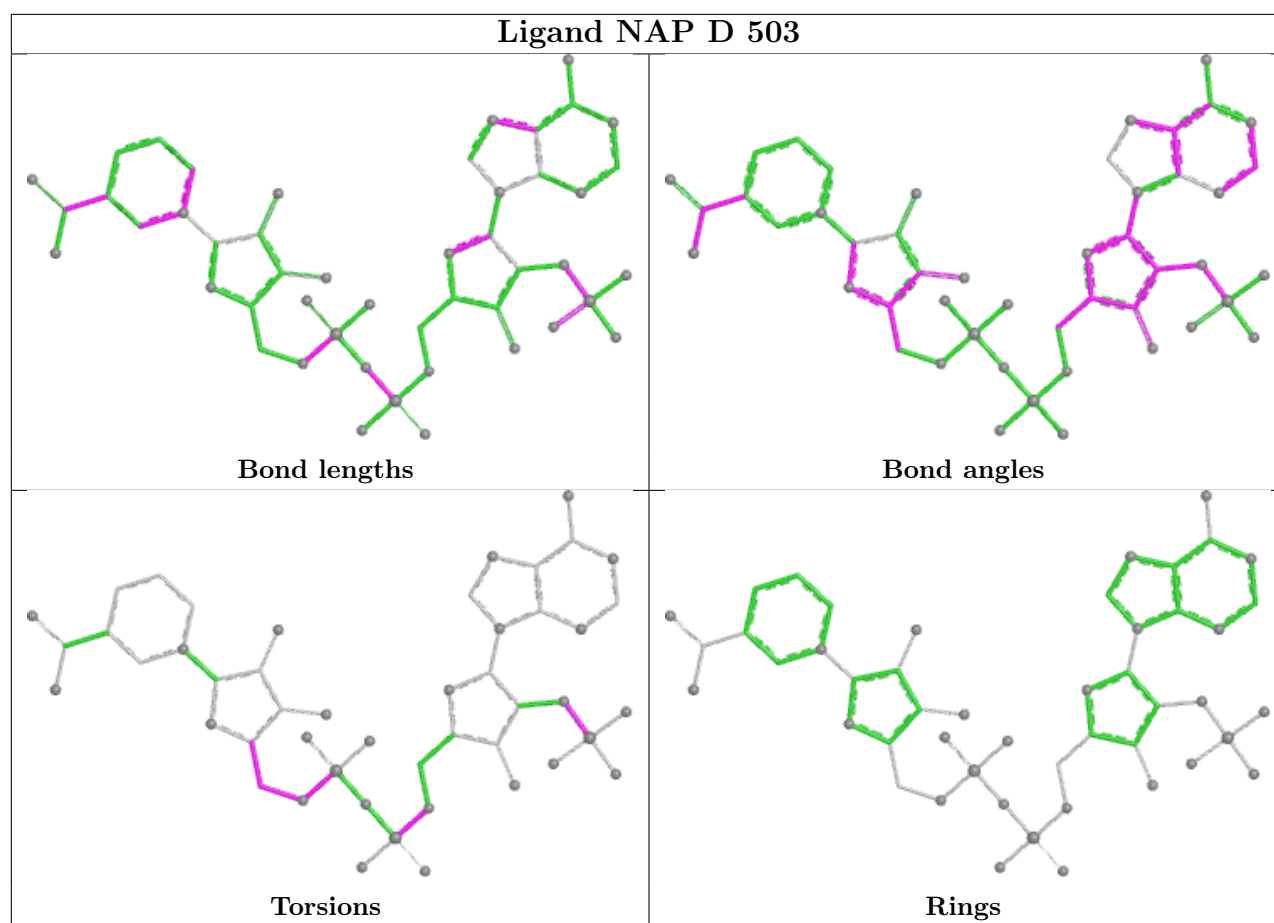
8 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	507	G3H	8	0
4	B	505	G3P	11	0
2	C	502	NAP	19	0
3	A	504	G3H	9	0
2	B	501	NAP	21	0
2	A	500	NAP	16	0
3	C	506	G3H	8	0
2	D	503	NAP	13	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 then 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.

Ligand NAP C 502

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 500

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP D 503

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.