



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 06:04 AM EDT

PDB ID : 2FR8  
Title : Structure of transhydrogenase (dI.R127A.NAD<sup>+</sup>)<sub>2</sub>(dIII.NADP<sup>+</sup>)<sub>1</sub> asymmetric complex  
Authors : Brondijk, T.H.; van Boxel, G.I.; Mather, O.C.; Quirk, P.G.; White, S.A.; Jackson, J.B.  
Deposited on : 2006-01-19  
Resolution : 2.60 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](mailto: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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

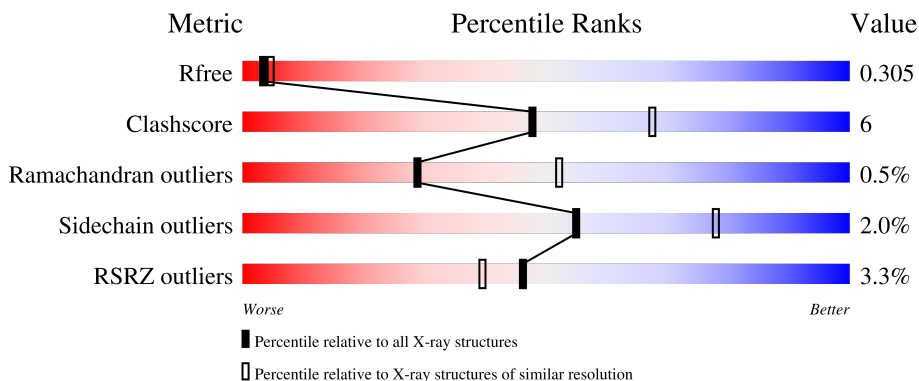
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


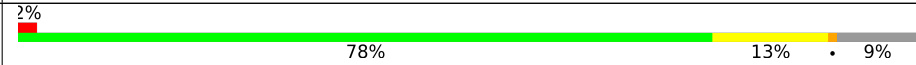
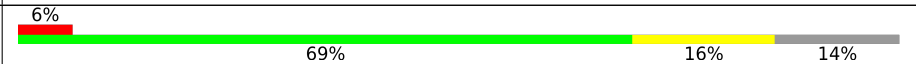
The reported resolution of this entry is 2.60 Å.

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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	384	 2% 78% 14% • 8%
1	B	384	 2% 78% 13% • 9%
2	C	203	 6% 69% 16% 14%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6599 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 NAD(P) transhydrogenase subunit alpha part 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	2590	1640	446	488	16	0	0	0
1	B	351	2567	1625	441	485	16	0	0	0

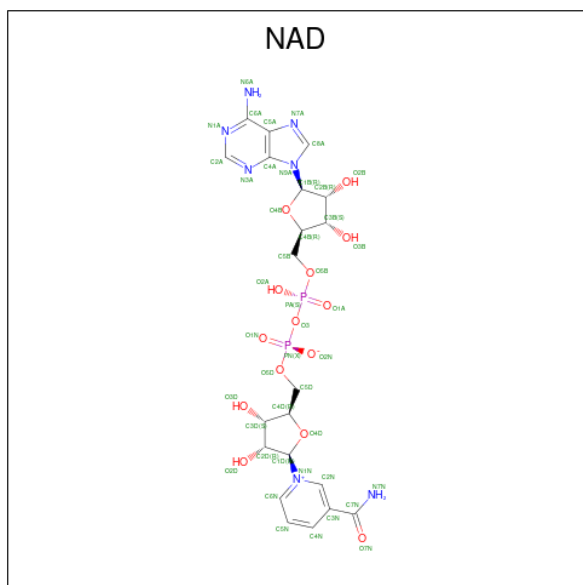
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	ARG	engineered mutation	UNP Q60164
B	127	ALA	ARG	engineered mutation	UNP Q60164

- Molecule 2 is a protein called NAD(P) transhydrogenase subunit beta.

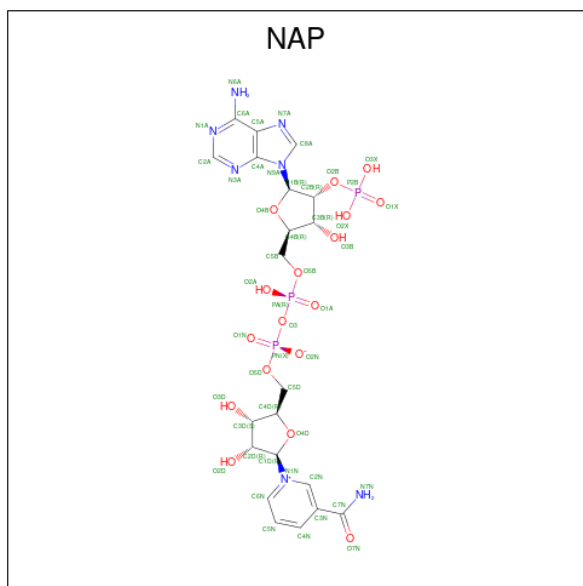
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	174	1311	830	217	253	11	0	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total 26	O 26	0	0
5	B	26	Total 26	O 26	0	0
5	C	4	Total 4	O 4	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.13Å 70.33Å 195.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.30 – 2.60 46.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (41.30-2.60) 98.6 (46.98-2.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.251 , 0.304 0.249 , 0.305	Depositor DCC
$R_{free}$ test set	1381 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtrriage
Anisotropy	0.304	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6599	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: NAD, 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	0.34	0/2624	0.59	0/3561
1	B	0.34	0/2599	0.60	0/3526
2	C	0.37	1/1334 (0.1%)	0.56	0/1803
All	All	0.35	1/6557 (0.0%)	0.58	0/8890

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	203	ASN	C-O	5.58	1.33	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	349	LYS	Peptide
1	B	350	ASP	Peptide



## 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	2590	0	2728	34	0
1	B	2567	0	2707	30	0
2	C	1311	0	1303	21	0
3	A	27	0	12	1	0
4	C	48	0	25	0	0
5	A	26	0	0	0	0
5	B	26	0	0	0	0
5	C	4	0	0	0	0
All	All	6599	0	6775	81	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 6.

All (81) 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:267:ILE:HG12	1:B:273:PRO:HD3	1.70	0.73
1:A:2:LYS:HE2	1:A:67:GLN:HE21	1.60	0.67
1:B:270:LYS:HB3	1:B:271:PRO:HD2	1.81	0.62
1:A:180:VAL:O	3:A:500:NAD:H4B	2.00	0.61
1:A:199:MET:HG2	1:A:217:LYS:HB2	1.82	0.61
1:A:13:GLU:OE1	1:A:75:GLN:NE2	2.35	0.60
1:A:303:LEU:HD13	1:A:317:ILE:HG13	1.85	0.59
1:A:163:MET:HG2	2:C:93:GLY:HA3	1.85	0.58
1:B:97:MET:HE1	1:B:342:PHE:HD2	1.68	0.58
1:B:293:LEU:HD22	1:B:323:VAL:HG21	1.86	0.58
1:B:350:ASP:O	1:B:351:THR:HG23	2.04	0.57
1:A:164:MET:HG3	2:C:84:ILE:HG21	1.86	0.57
1:A:181:GLY:O	1:A:185:LEU:HD12	2.04	0.57
1:A:156:PHE:CE2	1:A:158:ARG:HB2	2.40	0.56
2:C:63:GLN:HG2	2:C:98:LEU:HB3	1.87	0.56
1:A:165:THR:HB	1:A:168:GLY:O	2.05	0.56
1:A:180:VAL:HG21	1:A:207:THR:HG23	1.86	0.56
1:A:60:THR:HG23	1:A:63:GLN:H	1.72	0.54
1:B:5:ILE:HB	1:B:35:VAL:HG12	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:163:ILE:HG21	2:C:191:ALA:HA	1.89	0.54
2:C:50:ILE:HD12	2:C:125:ALA:HA	1.90	0.53
1:A:178:PHE:HB2	1:A:263:THR:HA	1.89	0.53
1:A:180:VAL:HG21	1:A:207:THR:CG2	2.38	0.53
2:C:164:LYS:O	2:C:188:PHE:HA	2.10	0.52
1:A:165:THR:HG22	1:A:167:ALA:H	1.73	0.52
2:C:138:ALA:HA	2:C:147:TYR:HA	1.92	0.52
1:B:13:GLU:OE1	1:B:75:GLN:NE2	2.43	0.51
1:B:142:ASN:HD21	1:B:186:GLN:HE21	1.58	0.51
1:B:47:ASP:HB3	1:B:57:ILE:HD13	1.92	0.51
1:B:270:LYS:HA	1:B:270:LYS:HE2	1.93	0.51
2:C:49:VAL:HG22	2:C:124:VAL:HB	1.93	0.50
1:B:2:LYS:HG2	1:B:32:GLU:HB3	1.92	0.50
1:A:158:ARG:HG3	1:B:329:ALA:HB3	1.93	0.50
1:A:1:MET:SD	1:A:1:MET:N	2.72	0.50
1:B:5:ILE:HG13	1:B:72:TRP:HB2	1.92	0.49
2:C:119:PHE:CE2	2:C:154:VAL:HG12	2.47	0.49
2:C:48:LYS:HA	2:C:79:GLU:HB3	1.94	0.49
1:A:116:LYS:HD2	1:A:372:GLY:HA3	1.93	0.49
1:B:38:GLY:HA2	1:B:41:VAL:HG23	1.95	0.48
1:A:156:PHE:CZ	1:A:158:ARG:HB2	2.49	0.47
1:A:273:PRO:HG2	1:A:275:LEU:HD11	1.97	0.47
2:C:85:HIS:CD2	2:C:133:VAL:HG13	2.49	0.47
1:A:164:MET:HG3	2:C:84:ILE:CG2	2.45	0.47
1:B:97:MET:CE	1:B:342:PHE:HD2	2.29	0.46
1:B:115:ARG:HB3	1:B:115:ARG:NH1	2.31	0.46
1:A:156:PHE:CZ	1:A:259:ASP:HB3	2.50	0.46
1:A:152:GLY:HA2	1:A:291:ILE:HD11	1.96	0.46
1:A:376:HIS:O	1:A:378:ALA:N	2.48	0.46
2:C:44:LYS:NZ	2:C:202:MET:O	2.48	0.46
2:C:38:ASP:HA	2:C:41:PHE:CD2	2.51	0.45
1:A:370:ARG:HH12	1:A:375:VAL:HG11	1.82	0.45
1:B:221:VAL:HG23	1:B:250:ALA:HB2	1.99	0.45
2:C:48:LYS:NZ	2:C:121:THR:OG1	2.49	0.45
2:C:164:LYS:NZ	2:C:168:ALA:O	2.37	0.45
1:B:156:PHE:CE2	1:B:158:ARG:HB2	2.52	0.44
2:C:73:LEU:HB3	2:C:78:VAL:HB	2.00	0.44
1:A:143:LEU:HD12	1:A:327:VAL:HG11	2.00	0.44
1:B:267:ILE:CG2	1:B:270:LYS:HB2	2.48	0.44
1:B:111:ALA:HA	1:B:114:LYS:HE2	2.00	0.44
1:A:5:ILE:HG13	1:A:72:TRP:HB2	2.00	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:MET:SD	1:A:254:GLU:HG3	2.58	0.43
1:A:327:VAL:HG12	1:A:330:ASP:HB2	2.01	0.43
1:A:142:ASN:O	1:A:186:GLN:HG2	2.18	0.43
2:C:50:ILE:HG22	2:C:81:SER:HB2	2.01	0.43
1:B:156:PHE:CD2	1:B:260:ILE:HD11	2.54	0.43
1:B:178:PHE:HB3	1:B:275:LEU:HD13	2.01	0.42
1:B:262:ILE:HD12	1:B:262:ILE:N	2.34	0.42
2:C:50:ILE:HD13	2:C:119:PHE:CE2	2.54	0.42
1:B:119:ALA:HB3	1:B:369:THR:HG22	2.01	0.42
1:A:178:PHE:HB3	1:A:275:LEU:HD22	2.01	0.42
1:B:343:LEU:HD11	1:B:354:LEU:HD13	2.01	0.42
1:A:156:PHE:CG	1:A:260:ILE:HD11	2.55	0.41
2:C:85:HIS:HE2	2:C:151:ILE:HA	1.84	0.41
1:B:113:THR:O	1:B:372:GLY:HA2	2.21	0.41
1:A:29:LEU:HD13	1:A:347:VAL:HG21	2.02	0.41
1:B:323:VAL:N	1:B:324:PRO:HD2	2.35	0.41
1:B:267:ILE:CG2	1:B:268:PRO:HD2	2.50	0.41
1:A:139:SER:CB	1:A:338:ASN:HD21	2.34	0.41
1:B:4:ALA:HA	1:B:34:ILE:O	2.21	0.41
2:C:85:HIS:HB3	2:C:88:ALA:HB2	2.02	0.40
1:B:156:PHE:CZ	1:B:259:ASP:HB3	2.56	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	350/384 (91%)	324 (93%)	25 (7%)	1 (0%)	41	64
1	B	347/384 (90%)	322 (93%)	22 (6%)	3 (1%)	17	35
2	C	172/203 (85%)	157 (91%)	15 (9%)	0	100	100
All	All	869/971 (90%)	803 (92%)	62 (7%)	4 (0%)	29	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	PRO
1	B	268	PRO
1	B	352	LYS
1	B	295	VAL

### 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	275/295 (93%)	268 (98%)	7 (2%)	47	73
1	B	273/295 (92%)	268 (98%)	5 (2%)	59	80
2	C	138/154 (90%)	136 (99%)	2 (1%)	67	85
All	All	686/744 (92%)	672 (98%)	14 (2%)	55	78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	65	LEU
1	A	163	MET
1	A	176	LEU
1	A	249	GLU
1	A	303	LEU
1	A	348	ASP
1	B	104	THR
1	B	147	ARG
1	B	194	LEU
1	B	279	GLU
1	B	295	VAL
2	C	63	GLN
2	C	91	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	75	GLN
1	A	338	ASN
1	B	75	GLN
1	B	142	ASN
2	C	61	GLN
2	C	63	GLN
2	C	197	GLN
2	C	203	ASN

### 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 monosaccharides 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$
3	NAD	A	500	-	24,29,48	1.23	2 (8%)	29,45,73	1.58	5 (17%)
4	NAP	C	400	-	45,52,52	1.69	3 (6%)	56,80,80	1.32	4 (7%)

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	NAD	A	500	-	-	1/12/32/62	0/3/3/5
4	NAP	C	400	-	-	14/31/67/67	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	400	NAP	O7N-C7N	8.78	1.41	1.24
3	A	500	NAD	C2A-N3A	3.99	1.38	1.32
4	C	400	NAP	C2A-N3A	3.68	1.38	1.32
4	C	400	NAP	C2A-N1A	2.52	1.38	1.33
3	A	500	NAD	C2A-N1A	2.12	1.37	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	400	NAP	N3A-C2A-N1A	-5.83	119.56	128.68
3	A	500	NAD	N3A-C2A-N1A	-5.56	120.00	128.68
4	C	400	NAP	C3N-C7N-N7N	3.89	122.42	117.75
3	A	500	NAD	PA-O3-PN	-3.15	122.01	132.83
3	A	500	NAD	C4A-C5A-N7A	-2.77	106.51	109.40
4	C	400	NAP	PN-O3-PA	-2.77	123.34	132.83
4	C	400	NAP	O7N-C7N-N7N	-2.61	118.88	122.58
3	A	500	NAD	O2N-PN-O1N	2.53	120.58	110.68
3	A	500	NAD	O4B-C1B-C2B	-2.47	103.32	106.93

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	400	NAP	C5B-O5B-PA-O1A
4	C	400	NAP	C5B-O5B-PA-O2A
4	C	400	NAP	O4D-C1D-N1N-C2N
4	C	400	NAP	O4B-C4B-C5B-O5B
4	C	400	NAP	C1B-C2B-O2B-P2B
4	C	400	NAP	C3B-C2B-O2B-P2B
4	C	400	NAP	C2B-O2B-P2B-O2X
4	C	400	NAP	C4D-C5D-O5D-PN
4	C	400	NAP	PN-O3-PA-O1A
4	C	400	NAP	C3B-C4B-C5B-O5B

*Continued on next page...*

Continued from previous page...

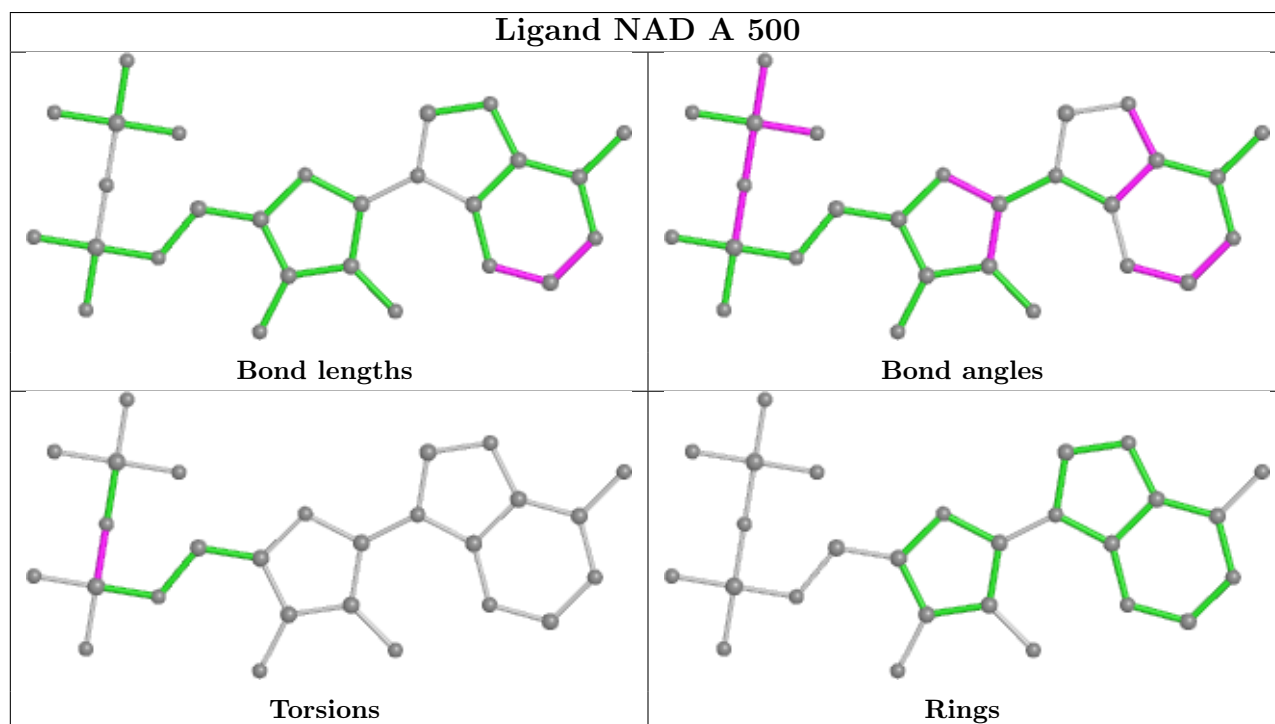
Mol	Chain	Res	Type	Atoms
4	C	400	NAP	O4D-C4D-C5D-O5D
4	C	400	NAP	PN-O3-PA-O2A
4	C	400	NAP	C5B-O5B-PA-O3
3	A	500	NAD	PN-O3-PA-O1A
4	C	400	NAP	PA-O3-PN-O2N

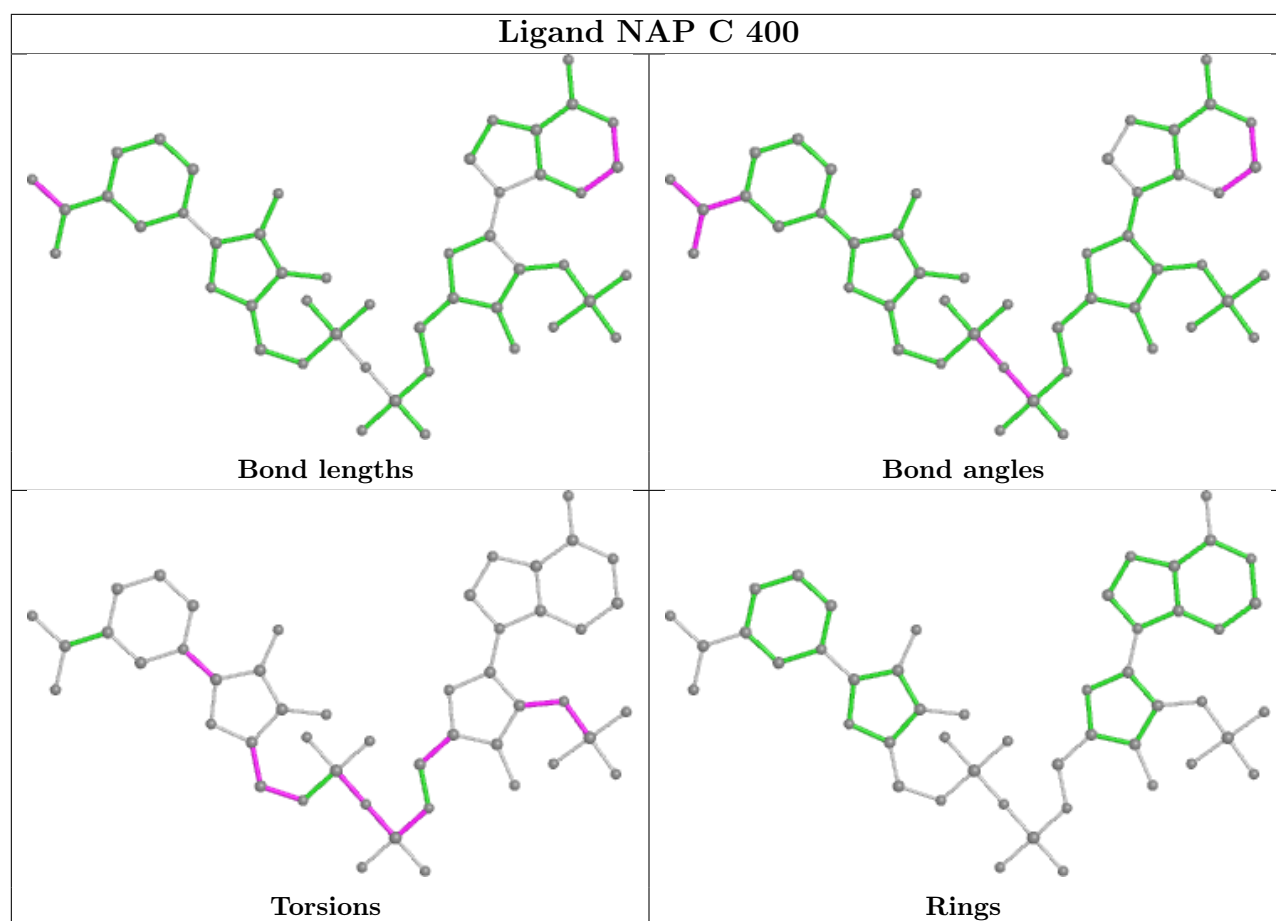
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	NAD	1	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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	354/384 (92%)	0.08	9 (2%) 57 51	30, 47, 71, 80	1 (0%)
1	B	351/384 (91%)	0.11	8 (2%) 60 54	33, 48, 67, 78	0
2	C	174/203 (85%)	0.42	12 (6%) 16 12	38, 54, 63, 65	0
All	All	879/971 (90%)	0.16	29 (3%) 46 39	30, 49, 69, 80	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268	PRO	8.7
1	A	350	ASP	4.8
1	A	348	ASP	4.4
1	A	349	LYS	4.0
2	C	189	GLY	3.2
1	B	349	LYS	3.2
1	B	350	ASP	2.9
2	C	188	PHE	2.8
2	C	50	ILE	2.7
2	C	138	ALA	2.7
2	C	130	ALA	2.7
2	C	177	GLU	2.7
2	C	140	THR	2.7
1	A	126	PRO	2.5
1	A	375	VAL	2.5
2	C	147	TYR	2.5
2	C	174	VAL	2.4
2	C	162	PHE	2.4
1	B	246	LYS	2.4
1	A	268	PRO	2.4
2	C	172	ALA	2.2
1	A	379	LEU	2.1
1	B	127	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	351	THR	2.1
2	C	146	ILE	2.1
1	B	269	GLY	2.1
1	A	218	PHE	2.1
1	B	249	GLU	2.1
1	A	220	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

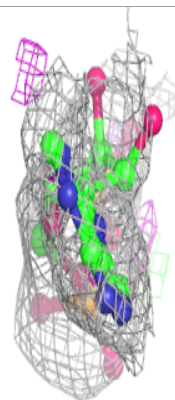
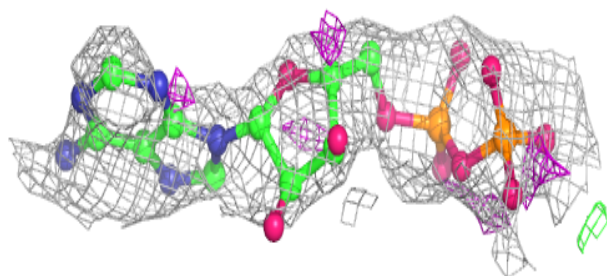
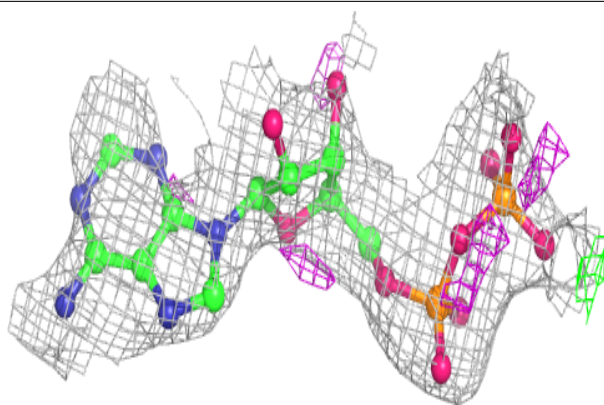
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAD	A	500	27/44	0.83	0.22	75,75,77,77	0
4	NAP	C	400	48/48	0.95	0.13	44,47,50,50	0

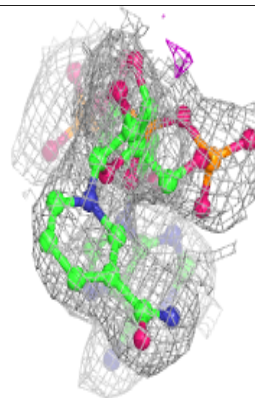
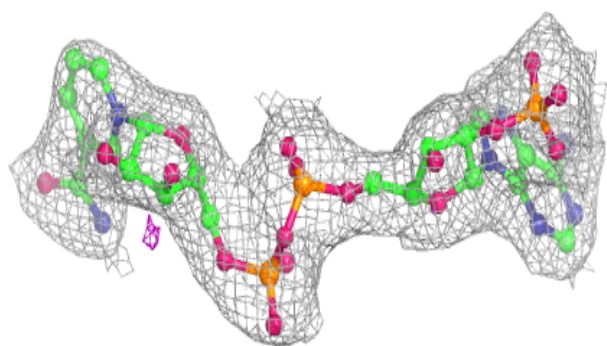
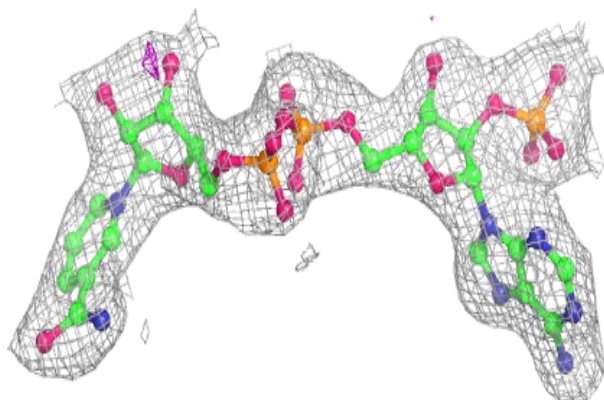
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around NAD A 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around NAP C 400:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.