



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:25 AM UTC

PDB ID : 4J16 / pdb_00004j16
Title : Crystal structure of Thermus thermophilus transhydrogenase heterotrimeric complex of the Alpha1 subunit dimer with the NADP binding domain (domain III) of the Beta subunit
Authors : Yamaguchi, M.; Leung, J.; Schurig Briccio, L.A.; Gennis, R.B.; Stout, C.D.
Deposited on : 2013-02-01
Resolution : 2.41 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)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

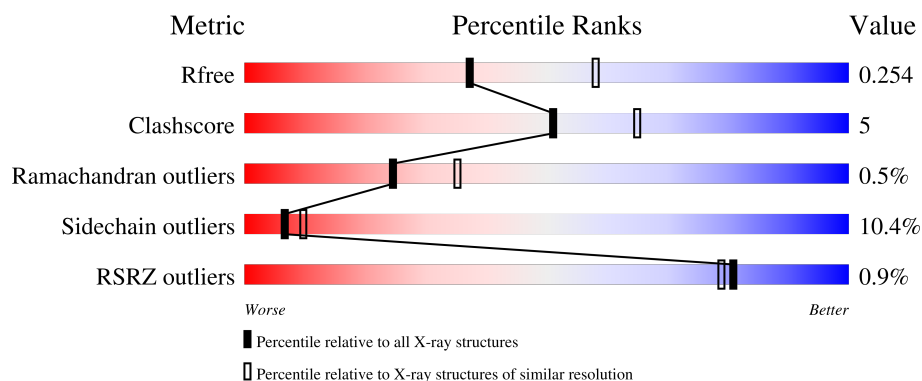
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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 $\leq 5\%$. 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	381	 81% 13% . .
1	B	381	 78% 15% . .
2	C	185	 83% 10% . .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7186 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/NADP transhydrogenase alpha subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2794	1772	498	512	12			
1	B	369	Total	C	N	O	S	0	0	0
			2769	1756	495	506	12			

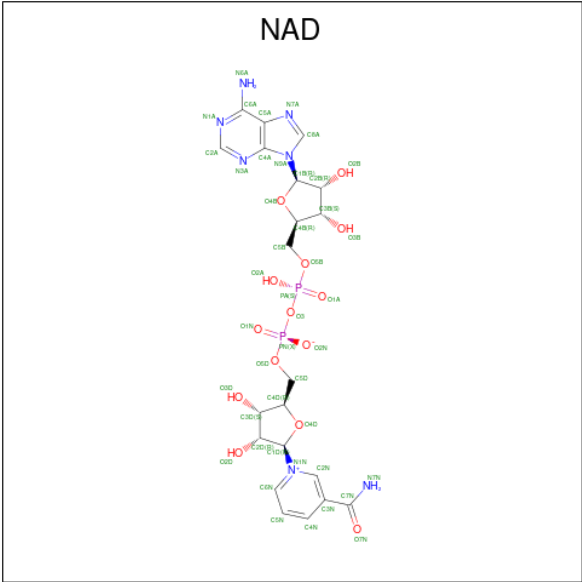
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q72GR8
A	-4	HIS	-	expression tag	UNP Q72GR8
A	-3	HIS	-	expression tag	UNP Q72GR8
A	-2	HIS	-	expression tag	UNP Q72GR8
A	-1	HIS	-	expression tag	UNP Q72GR8
A	0	HIS	-	expression tag	UNP Q72GR8
B	-5	HIS	-	expression tag	UNP Q72GR8
B	-4	HIS	-	expression tag	UNP Q72GR8
B	-3	HIS	-	expression tag	UNP Q72GR8
B	-2	HIS	-	expression tag	UNP Q72GR8
B	-1	HIS	-	expression tag	UNP Q72GR8
B	0	HIS	-	expression tag	UNP Q72GR8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	177	Total	C	N	O	S	0	0	0
			1343	860	229	248	6			

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).

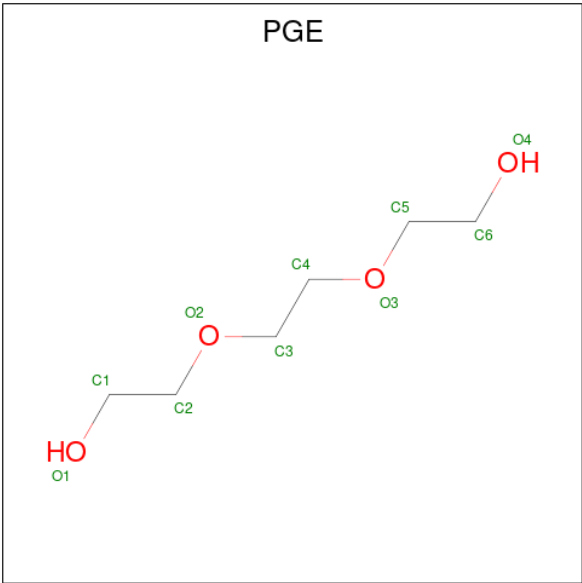


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

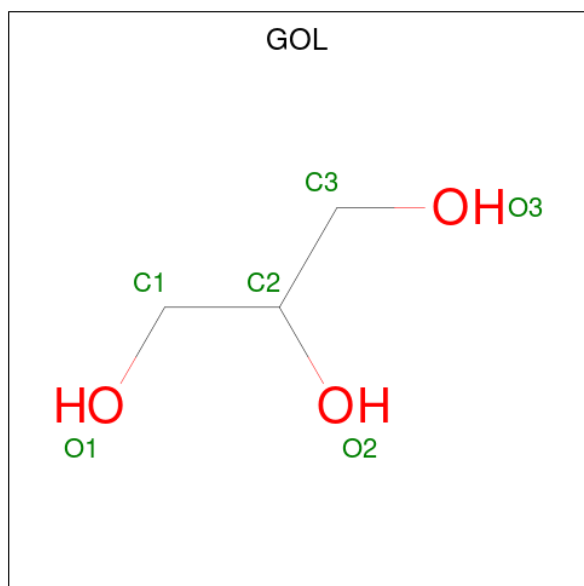
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



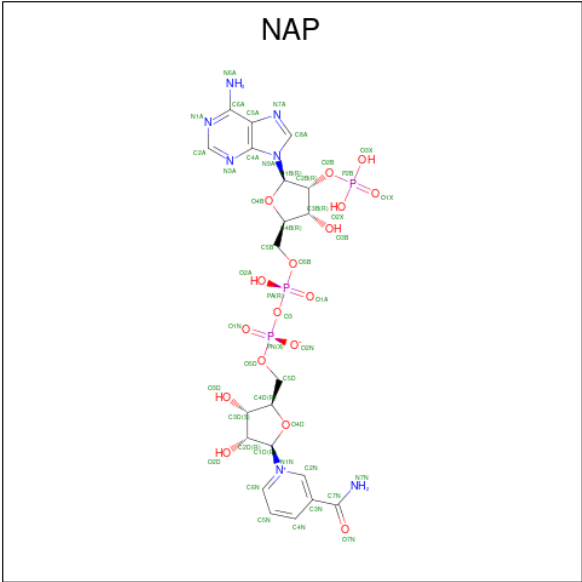
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 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
7	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

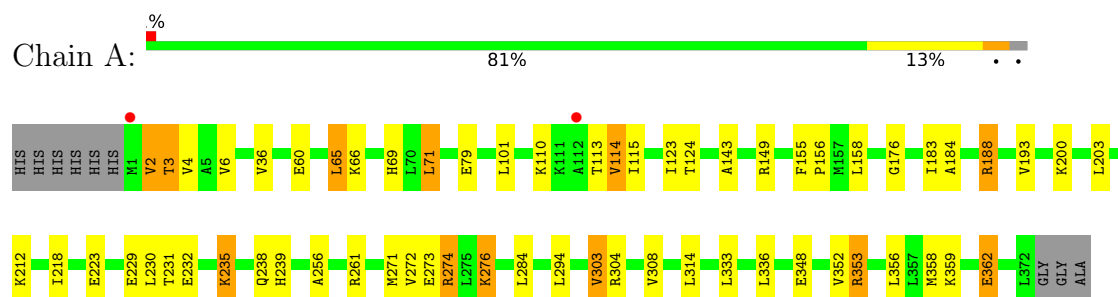
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	52	Total	O	0	0
			52	52		
8	B	35	Total	O	0	0
			35	35		
8	C	34	Total	O	0	0
			34	34		

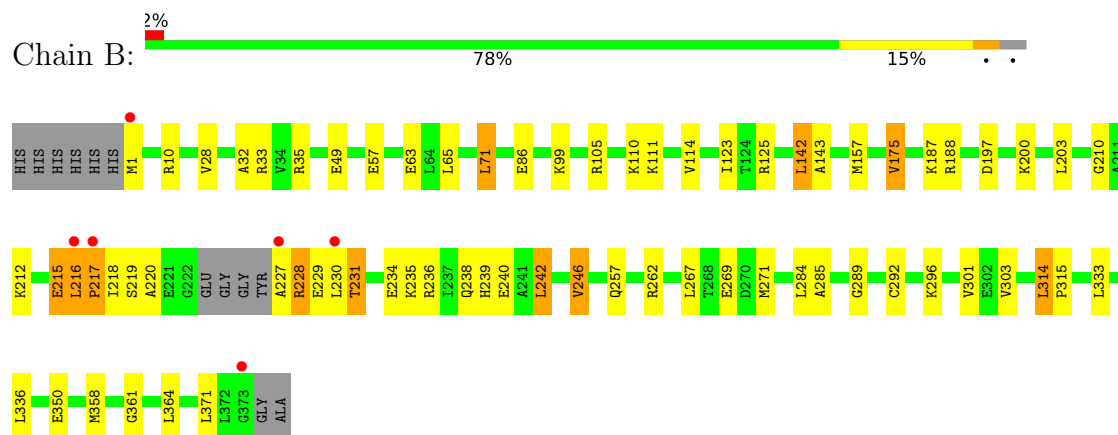
3 Residue-property plots

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 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.

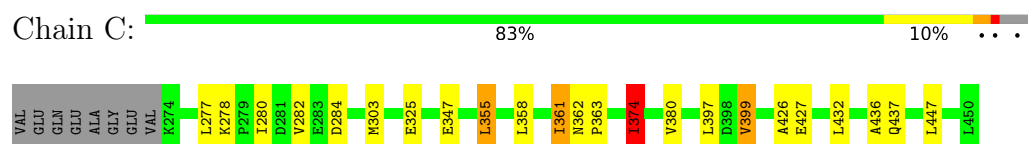
- Molecule 1: NAD/NADP transhydrogenase alpha subunit 1



- Molecule 1: NAD/NADP transhydrogenase alpha subunit 1



- Molecule 2: NAD(P) transhydrogenase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.62Å 75.04Å 198.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.98 – 2.41 39.98 – 2.41	Depositor EDS
% Data completeness (in resolution range)	96.3 (39.98-2.41) 96.5 (39.98-2.41)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.201 , 0.253 0.199 , 0.254	Depositor DCC
R_{free} test set	2007 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7186	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAD, CL, GOL, PGE, 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	0.57	0/2840	0.84	2/3852 (0.1%)
1	B	0.53	0/2813	0.80	1/3814 (0.0%)
2	C	0.59	0/1366	0.80	1/1848 (0.1%)
All	All	0.56	0/7019	0.82	4/9514 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	374	ILE	CB-CA-C	6.75	119.49	111.32
1	A	188	ARG	CB-CA-C	-6.07	100.71	110.79
1	B	220	ALA	N-CA-C	5.34	118.56	111.30
1	A	2	VAL	N-CA-C	5.30	120.37	109.34

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	2794	0	2911	29	0
1	B	2769	0	2892	35	0
2	C	1343	0	1378	11	0
3	A	44	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	44	0	26	2	0
4	B	1	0	0	0	0
5	B	10	0	14	2	0
6	B	6	0	8	2	0
6	C	6	0	8	0	0
7	C	48	0	25	0	0
8	A	52	0	0	0	0
8	B	35	0	0	0	0
8	C	34	0	0	1	0
All	All	7186	0	7288	74	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 5.

All (74) 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:216:LEU:HB3	1:B:217:PRO:HA	1.53	0.89
2:C:374:ILE:CD1	2:C:436:ALA:HB1	2.22	0.69
1:B:227:ALA:O	1:B:231:THR:HG23	1.96	0.66
1:B:175:VAL:HG23	1:B:197:ASP:HB2	1.79	0.63
1:B:216:LEU:CB	1:B:217:PRO:HA	2.28	0.63
2:C:374:ILE:HD11	2:C:436:ALA:HB1	1.80	0.61
1:A:353:ARG:HG3	1:A:353:ARG:HH21	1.66	0.60
1:B:114:VAL:HG12	1:B:358:MET:HG2	1.83	0.59
1:A:114:VAL:HG13	1:A:358:MET:HB2	1.85	0.57
1:A:272:VAL:HG11	1:A:294:LEU:HD11	1.86	0.56
1:B:143:ALA:HB2	1:B:284:LEU:HD11	1.87	0.56
1:A:274:ARG:HH11	1:A:274:ARG:HG3	1.69	0.56
1:B:215:GLU:HA	1:B:216:LEU:HD12	1.88	0.56
6:B:404:GOL:H2	2:C:347:GLU:HA	1.86	0.56
1:A:352:VAL:O	1:A:356:LEU:HB2	2.07	0.54
1:A:65:LEU:HD11	1:A:71:LEU:HG	1.90	0.54
2:C:278:LYS:NZ	2:C:426:ALA:O	2.40	0.54
1:A:176:GLY:HA3	3:A:500:NAD:H51N	1.90	0.53
1:B:187:LYS:HE2	1:B:210:GLY:O	2.08	0.53
1:A:273:GLU:HG2	1:A:304:ARG:HH22	1.74	0.53
1:B:285:ALA:O	1:B:289:GLY:O	2.28	0.52
1:A:113:THR:HG23	1:A:359:LYS:HA	1.93	0.51
1:A:353:ARG:HH21	1:A:353:ARG:CG	2.24	0.51
1:A:294:LEU:HD13	1:A:303:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:282:VAL:HG13	8:C:618:HOH:O	2.12	0.49
2:C:280:ILE:HG12	2:C:284:ASP:HB2	1.93	0.49
1:B:114:VAL:HG12	1:B:358:MET:CG	2.43	0.49
1:B:242:LEU:O	1:B:246:VAL:HB	2.13	0.49
1:B:111:LYS:HA	1:B:361:GLY:CA	2.43	0.49
2:C:358:LEU:HA	2:C:361:ILE:HG22	1.95	0.49
1:B:216:LEU:HB3	1:B:217:PRO:CA	2.35	0.49
1:A:2:VAL:HG23	1:A:69:HIS:HB2	1.95	0.48
1:B:215:GLU:C	1:B:216:LEU:HD12	2.39	0.48
1:B:111:LYS:HA	1:B:361:GLY:HA3	1.96	0.47
1:B:216:LEU:CB	1:B:217:PRO:CA	2.91	0.47
1:B:227:ALA:HB1	1:B:231:THR:CG2	2.44	0.47
1:B:238:GLN:O	1:B:242:LEU:HG	2.14	0.47
1:A:143:ALA:HB2	1:A:284:LEU:HD11	1.97	0.46
1:B:157:MET:CE	2:C:355:LEU:HD23	2.45	0.46
1:B:219:SER:HB3	1:B:229:GLU:OE1	2.16	0.46
1:A:274:ARG:HH11	1:A:274:ARG:CG	2.28	0.46
1:B:257:GLN:H	3:B:401:NAD:H52A	1.80	0.46
1:B:314:LEU:N	1:B:315:PRO:CD	2.78	0.46
1:A:155:PHE:N	1:A:156:PRO:HD2	2.30	0.46
1:B:65:LEU:HD21	1:B:71:LEU:HG	1.97	0.45
2:C:380:VAL:HB	2:C:399:VAL:HG11	1.98	0.45
1:B:227:ALA:HB1	1:B:231:THR:HG23	1.98	0.44
1:A:231:THR:O	1:A:235:LYS:HB2	2.17	0.44
2:C:362:ASN:N	2:C:363:PRO:HD2	2.33	0.44
1:B:35:ARG:NH1	1:B:63:GLU:O	2.51	0.44
5:B:403:PGE:H2	5:B:403:PGE:H42	1.72	0.44
1:A:188:ARG:HG2	6:B:404:GOL:H32	2.00	0.43
1:A:2:VAL:HG22	1:A:3:THR:N	2.33	0.43
1:B:33:ARG:NH2	1:B:57:GLU:OE1	2.52	0.43
1:A:294:LEU:HD12	1:A:308:VAL:HG21	2.02	0.42
1:B:296:LYS:HG3	1:B:301:VAL:HG11	2.01	0.42
1:A:256:ALA:HB1	3:A:500:NAD:H52A	2.02	0.42
1:B:234:GLU:O	1:B:236:ARG:N	2.53	0.42
1:A:6:VAL:CG1	1:A:36:VAL:HG22	2.49	0.41
1:A:188:ARG:HB3	1:B:188:ARG:O	2.20	0.41
1:A:239:HIS:CE1	1:A:271:MET:HE3	2.54	0.41
1:A:183:ILE:HG23	1:A:193:VAL:HG11	2.02	0.41
1:B:267:LEU:HB2	1:B:292:CYS:HA	2.02	0.41
1:B:28:VAL:HA	1:B:32:ALA:O	2.20	0.41
3:B:401:NAD:H51N	5:B:403:PGE:H22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ALA:O	1:A:188:ARG:HG3	2.21	0.41
1:A:188:ARG:HD3	1:B:188:ARG:O	2.21	0.41
1:A:218:ILE:O	1:A:238:GLN:NE2	2.53	0.41
1:A:358:MET:HA	1:A:362:GLU:O	2.20	0.41
1:B:239:HIS:HA	1:B:271:MET:CE	2.50	0.41
1:B:200:LYS:CE	1:B:216:LEU:HD23	2.50	0.41
1:A:276:LYS:HB3	1:A:276:LYS:HE2	1.91	0.40
1:B:142:LEU:HB3	1:B:314:LEU:HG	2.03	0.40
2:C:303:MET:HB2	2:C:374:ILE:HG13	2.03	0.40

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	370/381 (97%)	352 (95%)	18 (5%)	0	100	100
1	B	365/381 (96%)	345 (94%)	15 (4%)	5 (1%)	9	12
2	C	175/185 (95%)	172 (98%)	3 (2%)	0	100	100
All	All	910/947 (96%)	869 (96%)	36 (4%)	5 (0%)	24	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	216	LEU
1	B	228	ARG
1	B	235	LYS
1	B	217	PRO
1	B	215	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	287/293 (98%)	254 (88%)	33 (12%)	5	7
1	B	285/293 (97%)	255 (90%)	30 (10%)	6	9
2	C	139/146 (95%)	128 (92%)	11 (8%)	11	18
All	All	711/732 (97%)	637 (90%)	74 (10%)	7	10

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	4	VAL
1	A	60	GLU
1	A	65	LEU
1	A	66	LYS
1	A	71	LEU
1	A	79	GLU
1	A	101	LEU
1	A	110	LYS
1	A	114	VAL
1	A	115	ILE
1	A	123	ILE
1	A	124	THR
1	A	149	ARG
1	A	158	LEU
1	A	200	LYS
1	A	203	LEU
1	A	212	LYS
1	A	223	GLU
1	A	229	GLU
1	A	230	LEU
1	A	232	GLU
1	A	235	LYS
1	A	261	ARG
1	A	274	ARG
1	A	276	LYS

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Mol	Chain	Res	Type
1	A	303	VAL
1	A	314	LEU
1	A	333	LEU
1	A	336	LEU
1	A	348	GLU
1	A	353	ARG
1	A	362	GLU
1	B	1	MET
1	B	10	ARG
1	B	49	GLU
1	B	71	LEU
1	B	86	GLU
1	B	99	LYS
1	B	105	ARG
1	B	110	LYS
1	B	123	ILE
1	B	125	ARG
1	B	142	LEU
1	B	175	VAL
1	B	203	LEU
1	B	212	LYS
1	B	218	ILE
1	B	228	ARG
1	B	230	LEU
1	B	231	THR
1	B	240	GLU
1	B	242	LEU
1	B	246	VAL
1	B	262	ARG
1	B	269	GLU
1	B	303	VAL
1	B	314	LEU
1	B	333	LEU
1	B	336	LEU
1	B	350	GLU
1	B	364	LEU
1	B	371	LEU
2	C	277	LEU
2	C	325	GLU
2	C	355	LEU
2	C	361	ILE
2	C	374	ILE

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Mol	Chain	Res	Type
2	C	397	LEU
2	C	399	VAL
2	C	427	GLU
2	C	432	LEU
2	C	437	GLN
2	C	447	LEU

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	69	HIS
1	A	75	GLN
1	A	83	GLN
1	A	98	HIS
1	A	313	ASN
1	A	329	ASN
1	B	108	GLN
1	B	257	GLN
1	B	321	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](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	$\# Z > 2$
6	GOL	B	404	-	5,5,5	0.48	0	5,5,5	0.94	0
6	GOL	C	502	-	5,5,5	0.45	0	5,5,5	0.39	0
5	PGE	B	403	-	9,9,9	0.65	0	8,8,8	0.45	0
3	NAD	B	401	-	46,48,48	1.57	5 (10%)	64,73,73	1.92	16 (25%)
7	NAP	C	501	-	50,52,52	1.68	11 (22%)	71,80,80	2.25	21 (29%)
3	NAD	A	500	-	46,48,48	1.78	7 (15%)	64,73,73	1.86	12 (18%)

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
6	GOL	B	404	-	-	2/4/4/4	-
6	GOL	C	502	-	-	4/4/4/4	-
5	PGE	B	403	-	-	5/7/7/7	-
3	NAD	B	401	-	-	2/30/62/62	0/5/5/5
7	NAP	C	501	-	-	8/35/67/67	0/5/5/5
3	NAD	A	500	-	-	12/30/62/62	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	NAD	PA-O3	5.93	1.65	1.59
3	A	500	NAD	PN-O3	5.29	1.65	1.59
3	B	401	NAD	PA-O3	4.86	1.64	1.59
3	B	401	NAD	PN-O3	4.79	1.64	1.59
7	C	501	NAP	PN-O3	4.73	1.64	1.59
7	C	501	NAP	P2B-O1X	4.64	1.64	1.50
3	A	500	NAD	PA-O1A	4.38	1.66	1.50
3	A	500	NAD	PN-O1N	4.34	1.65	1.50
7	C	501	NAP	PN-O1N	4.14	1.65	1.50
3	B	401	NAD	PA-O1A	4.03	1.64	1.50
3	B	401	NAD	PN-O1N	3.99	1.64	1.50
7	C	501	NAP	PA-O1A	3.38	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	501	NAP	PA-O3	3.28	1.63	1.59
3	A	500	NAD	O4D-C1D	2.68	1.44	1.40
7	C	501	NAP	P2B-O3X	2.65	1.64	1.54
7	C	501	NAP	P2B-O2X	2.46	1.63	1.54
7	C	501	NAP	P2B-O2B	2.39	1.63	1.59
3	B	401	NAD	O4D-C1D	2.20	1.43	1.40
3	A	500	NAD	PA-O2A	2.18	1.65	1.55
7	C	501	NAP	C5A-N7A	-2.17	1.35	1.39
3	A	500	NAD	PN-O2N	2.09	1.65	1.55
7	C	501	NAP	PA-O2A	2.09	1.65	1.55
7	C	501	NAP	PN-O2N	2.05	1.64	1.55

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	501	NAP	C3N-C7N-N7N	7.00	126.36	117.74
3	A	500	NAD	C5A-C4A-N3A	-6.68	117.52	126.72
3	B	401	NAD	C5A-C4A-N3A	-6.32	118.02	126.72
7	C	501	NAP	N3A-C2A-N1A	-5.73	119.92	128.58
7	C	501	NAP	C4D-O4D-C1D	5.26	114.74	109.92
7	C	501	NAP	C5A-C4A-N3A	-4.93	119.93	126.72
3	A	500	NAD	O4B-C1B-N9A	4.83	117.38	108.09
7	C	501	NAP	C2B-C1B-N9A	-4.65	106.10	113.75
3	A	500	NAD	N3A-C2A-N1A	-4.49	121.79	128.58
3	B	401	NAD	N3A-C4A-N9A	4.25	134.39	127.17
3	A	500	NAD	N3A-C4A-N9A	4.23	134.36	127.17
3	B	401	NAD	O4B-C1B-N9A	4.19	116.14	108.09
3	B	401	NAD	N3A-C2A-N1A	-4.19	122.24	128.58
7	C	501	NAP	O3B-C3B-C4B	-4.13	99.21	111.08
3	A	500	NAD	C2A-N3A-C4A	4.05	121.72	111.83
7	C	501	NAP	C2A-N3A-C4A	3.86	121.25	111.83
3	A	500	NAD	C4A-C5A-N7A	-3.81	106.22	110.58
3	B	401	NAD	C4A-C5A-N7A	-3.72	106.33	110.58
7	C	501	NAP	O7N-C7N-C3N	-3.71	115.06	119.60
3	B	401	NAD	C2A-N3A-C4A	3.69	120.83	111.83
3	B	401	NAD	C5A-N7A-C8A	3.53	109.00	103.45
3	B	401	NAD	N9A-C8A-N7A	-3.47	109.02	113.94
7	C	501	NAP	C4A-C5A-N7A	-3.43	106.66	110.58
3	A	500	NAD	C5A-N7A-C8A	3.43	108.83	103.45
7	C	501	NAP	N9A-C8A-N7A	-3.40	109.11	113.94
7	C	501	NAP	C5A-N7A-C8A	3.35	108.72	103.45
3	B	401	NAD	C4D-O4D-C1D	-3.33	106.87	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	501	NAP	O3D-C3D-C4D	-3.26	101.71	111.08
7	C	501	NAP	O4B-C4B-C3B	-3.24	98.72	105.15
7	C	501	NAP	N3A-C4A-N9A	3.11	132.46	127.17
3	A	500	NAD	N9A-C8A-N7A	-2.99	109.69	113.94
3	B	401	NAD	C2B-C1B-N9A	-2.92	106.04	113.30
7	C	501	NAP	O4B-C1B-C2B	-2.89	101.61	106.59
7	C	501	NAP	C2B-C3B-C4B	2.88	108.18	101.99
7	C	501	NAP	O7N-C7N-N7N	-2.80	118.57	122.62
7	C	501	NAP	C6N-N1N-C2N	-2.78	119.52	121.88
3	B	401	NAD	O4B-C4B-C5B	-2.46	101.46	109.33
7	C	501	NAP	O2D-C2D-C3D	-2.32	104.37	111.82
3	B	401	NAD	C5D-C4D-C3D	-2.30	106.95	115.21
3	B	401	NAD	C5N-C4N-C3N	-2.21	118.19	120.36
3	B	401	NAD	C4A-N9A-C8A	2.21	108.06	105.74
3	A	500	NAD	C2B-C1B-N9A	-2.20	107.85	113.30
3	B	401	NAD	C5B-C4B-C3B	-2.19	107.31	115.21
3	A	500	NAD	C5N-C4N-C3N	-2.18	118.22	120.36
3	A	500	NAD	C6N-N1N-C2N	-2.18	120.02	121.88
3	A	500	NAD	C5A-C4A-N9A	2.12	108.12	105.81
7	C	501	NAP	O2A-PA-O1A	2.10	122.22	112.44
7	C	501	NAP	C4A-N9A-C8A	2.05	107.89	105.74
3	B	401	NAD	O2N-PN-O1N	2.01	121.79	112.44

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	NAD	C5D-O5D-PN-O3
3	A	500	NAD	C2D-C1D-N1N-C2N
3	A	500	NAD	C2D-C1D-N1N-C6N
6	B	404	GOL	O1-C1-C2-C3
6	C	502	GOL	O1-C1-C2-O2
6	C	502	GOL	O1-C1-C2-C3
6	C	502	GOL	C1-C2-C3-O3
7	C	501	NAP	O4D-C1D-N1N-C2N
7	C	501	NAP	O4D-C1D-N1N-C6N
7	C	501	NAP	C2D-C1D-N1N-C2N
7	C	501	NAP	C2D-C1D-N1N-C6N
3	B	401	NAD	O4B-C4B-C5B-O5B
3	B	401	NAD	C3B-C4B-C5B-O5B
5	B	403	PGE	C4-C3-O2-C2
5	B	403	PGE	O1-C1-C2-O2

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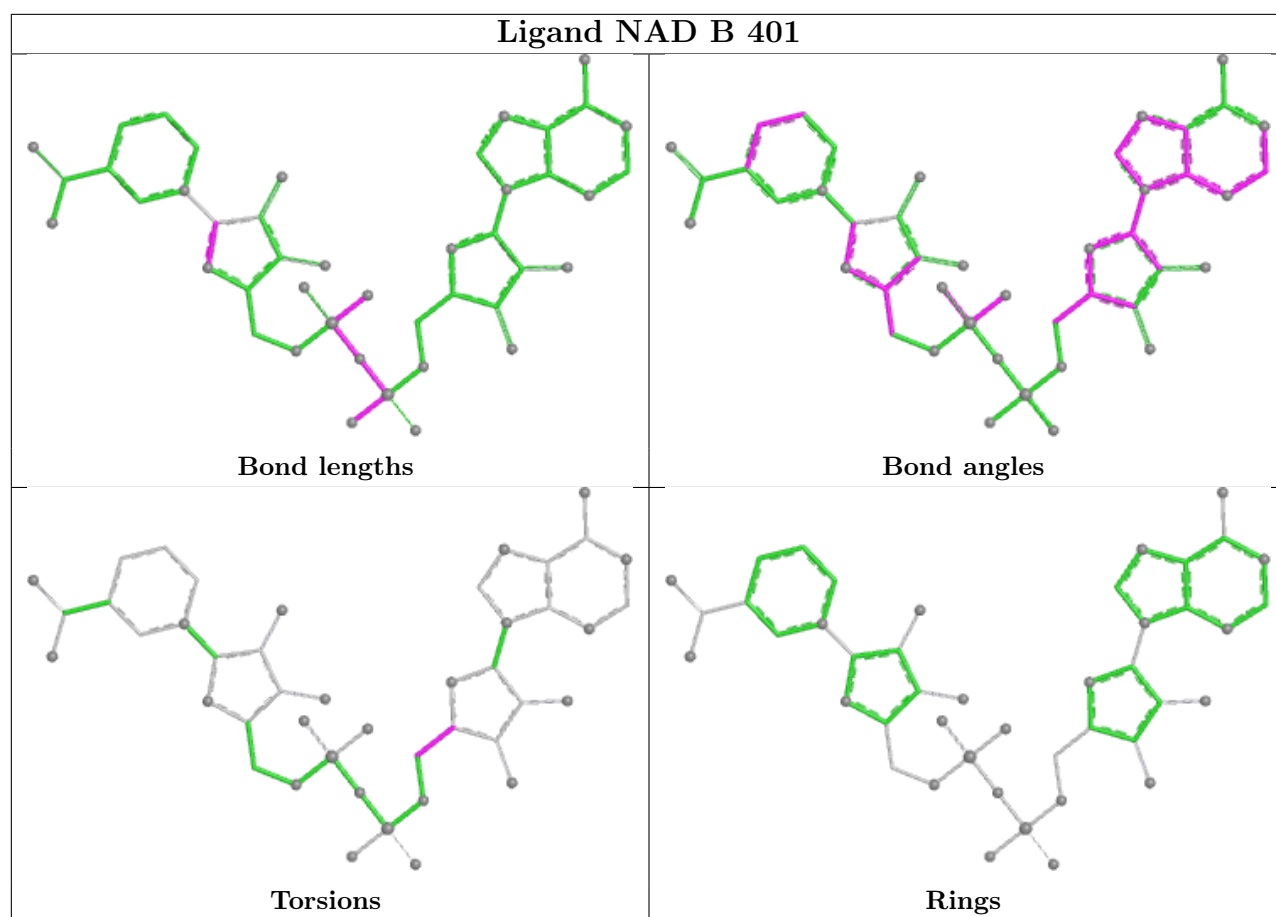
Mol	Chain	Res	Type	Atoms
6	B	404	GOL	O1-C1-C2-O2
6	C	502	GOL	O2-C2-C3-O3
3	A	500	NAD	C3B-C4B-C5B-O5B
3	A	500	NAD	O4B-C4B-C5B-O5B
3	A	500	NAD	O4D-C4D-C5D-O5D
5	B	403	PGE	C1-C2-O2-C3
7	C	501	NAP	PN-O3-PA-O1A
3	A	500	NAD	C5D-O5D-PN-O1N
3	A	500	NAD	C4B-C5B-O5B-PA
3	A	500	NAD	PN-O3-PA-O1A
5	B	403	PGE	C6-C5-O3-C4
5	B	403	PGE	C3-C4-O3-C5
3	A	500	NAD	C3D-C4D-C5D-O5D
7	C	501	NAP	C3B-C4B-C5B-O5B
3	A	500	NAD	PN-O3-PA-O2A
7	C	501	NAP	PN-O3-PA-O2A
3	A	500	NAD	C4D-C5D-O5D-PN
7	C	501	NAP	C1B-C2B-O2B-P2B

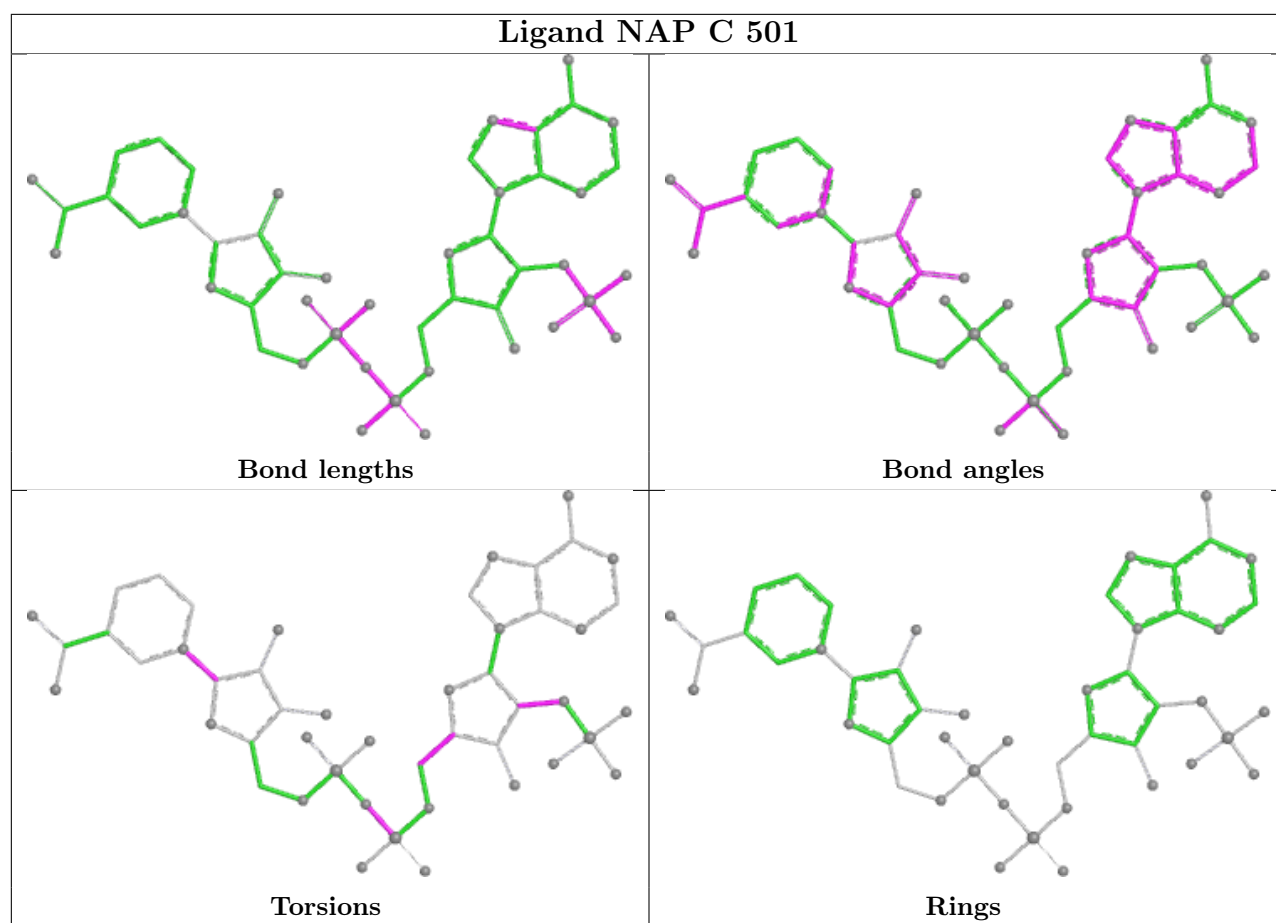
There are no ring outliers.

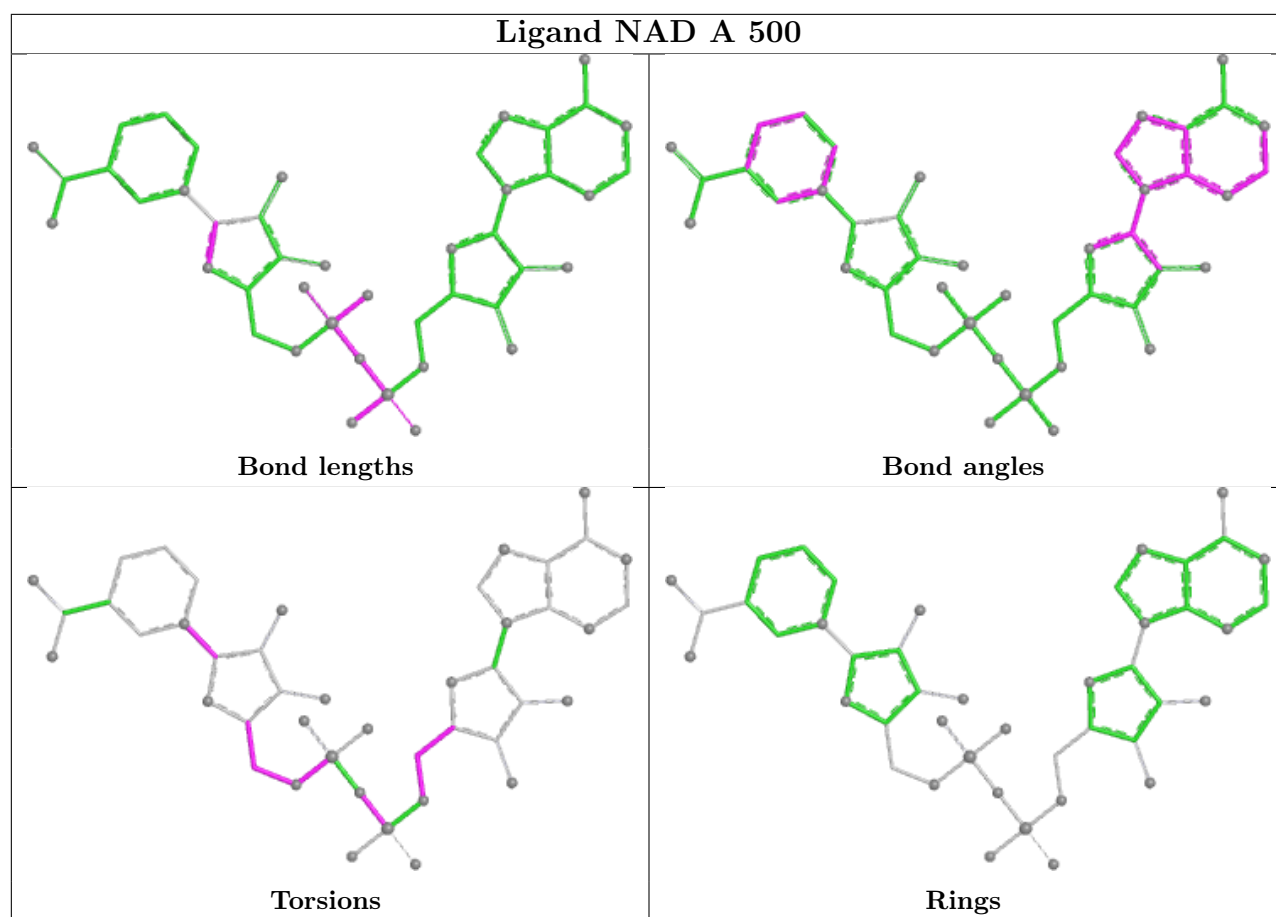
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	404	GOL	2	0
5	B	403	PGE	2	0
3	B	401	NAD	2	0
3	A	500	NAD	2	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 [i](#)

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

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, 95th 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 ²)	Q<0.9
1	A	372/381 (97%)	-0.08	2 (0%) 87 86	39, 70, 103, 120	0
1	B	369/381 (96%)	0.07	6 (1%) 70 67	42, 77, 114, 146	0
2	C	177/185 (95%)	-0.29	0 100 100	40, 59, 79, 96	0
All	All	918/947 (96%)	-0.06	8 (0%) 81 79	39, 69, 107, 146	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	ALA	4.5
1	B	230	LEU	3.6
1	B	216	LEU	2.6
1	B	217	PRO	2.4
1	A	1	MET	2.2
1	A	112	ALA	2.1
1	B	1	MET	2.1
1	B	373	GLY	2.1

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 oligosaccharides in this entry.

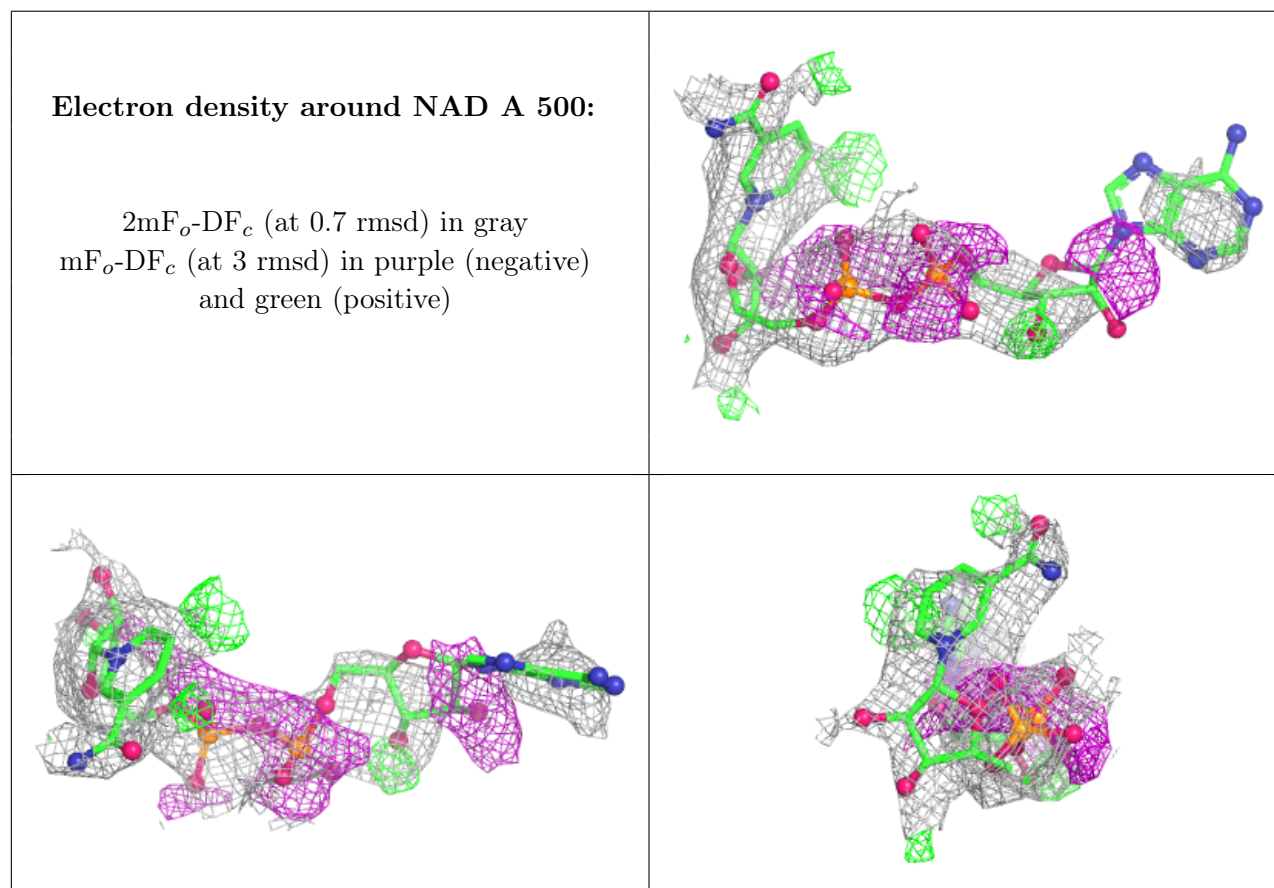
6.4 Ligands [i](#)

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, 95th 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.

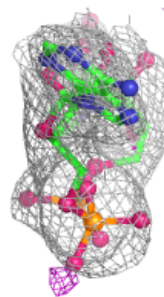
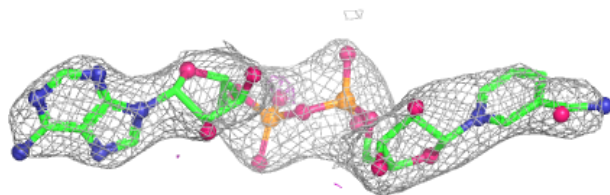
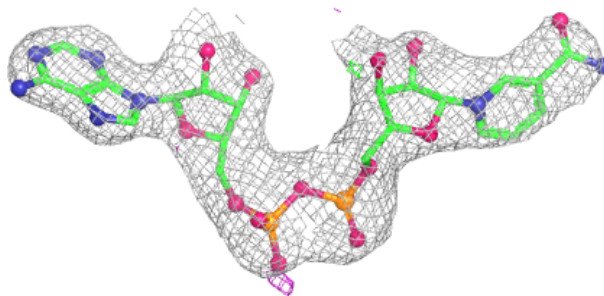
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAD	A	500	44/44	0.72	0.17	103,120,160,164	0
6	GOL	B	404	6/6	0.83	0.19	53,57,60,61	0
5	PGE	B	403	10/10	0.86	0.13	65,72,75,78	0
6	GOL	C	502	6/6	0.89	0.13	83,89,90,92	0
4	CL	B	402	1/1	0.91	0.17	83,83,83,83	0
3	NAD	B	401	44/44	0.94	0.08	67,76,91,94	0
7	NAP	C	501	48/48	0.98	0.05	43,47,60,63	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.

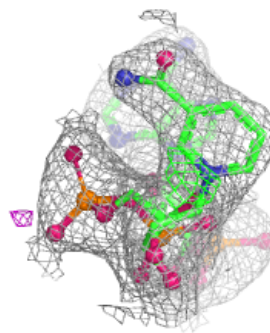
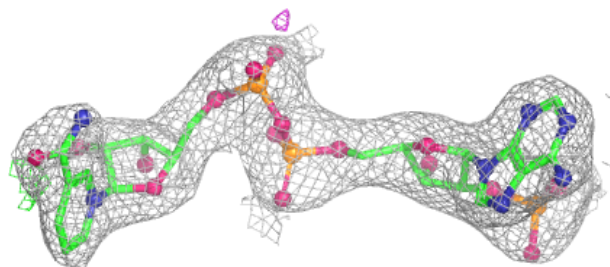
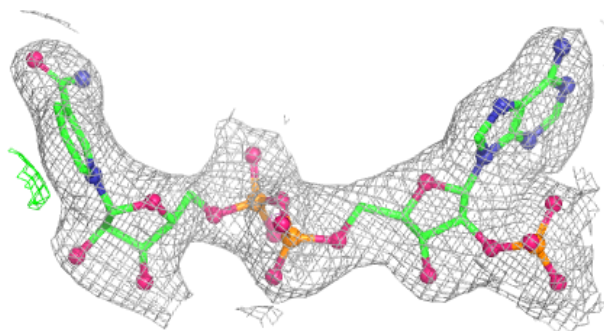


Electron density around NAD B 401:

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

**Electron density around NAP C 501:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.