



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:48 pm BST

PDB ID : 5Z75
Title : Artificial L-threonine 3-dehydrogenase designed by ancestral sequence reconstruction.
Authors : Nakano, S.; Motoyama, T.; Miyashita, Y.; Ishizuka, Y.; Matsuo, N.; Tokiwa, H.; Shinoda, S.; Asano, Y.; Ito, S.
Deposited on : 2018-01-27
Resolution : 2.10 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 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 : 2.11
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) : 2.11

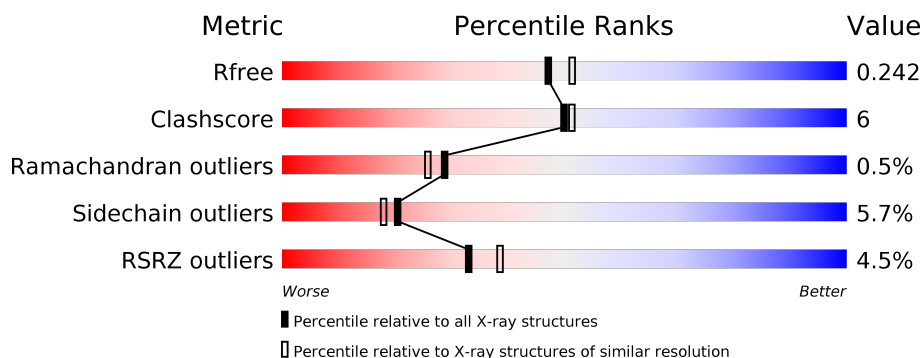
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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.

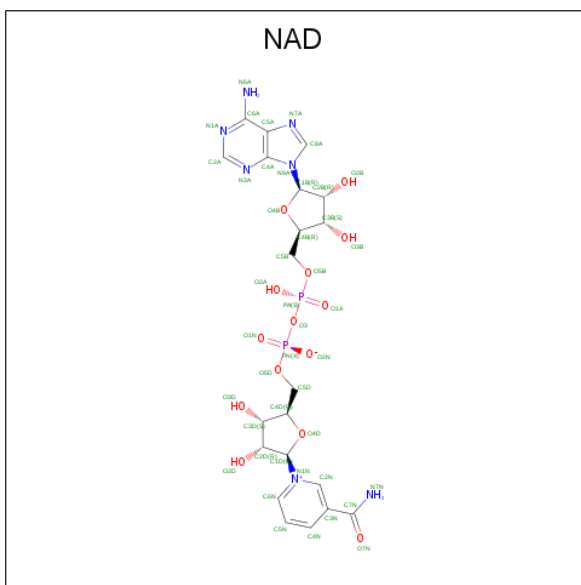
Mol	Chain	Length	Quality of chain
1	A	327	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 6%</div> </div> </div>
1	B	327	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>• 6%</div> </div> </div>
1	C	327	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• 6%</div> </div> </div>
1	D	327	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• 6%</div> </div> </div>

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 Artificial L-threonine 3-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total 2439	C 1555	N 395	O 474	S 15	0	0	0
1	B	306	Total 2437	C 1554	N 394	O 475	S 14	0	0	0
1	C	306	Total 2437	C 1554	N 394	O 475	S 14	0	0	0
1	D	306	Total 2437	C 1554	N 394	O 475	S 14	0	0	0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $\text{C}_{21}\text{H}_{27}\text{N}_7\text{O}_{14}\text{P}_2$).



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

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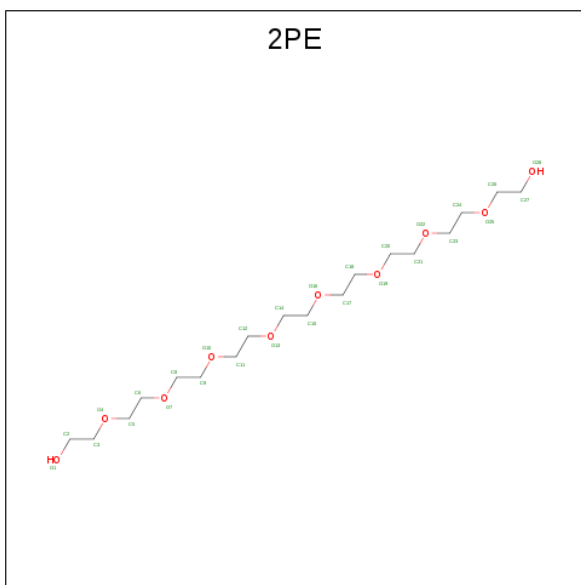
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: C₁₈H₃₈O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 28	C 18	O 10	0	0
4	C	1	Total 28	C 18	O 10	0	0
4	D	1	Total 28	C 18	O 10	0	0

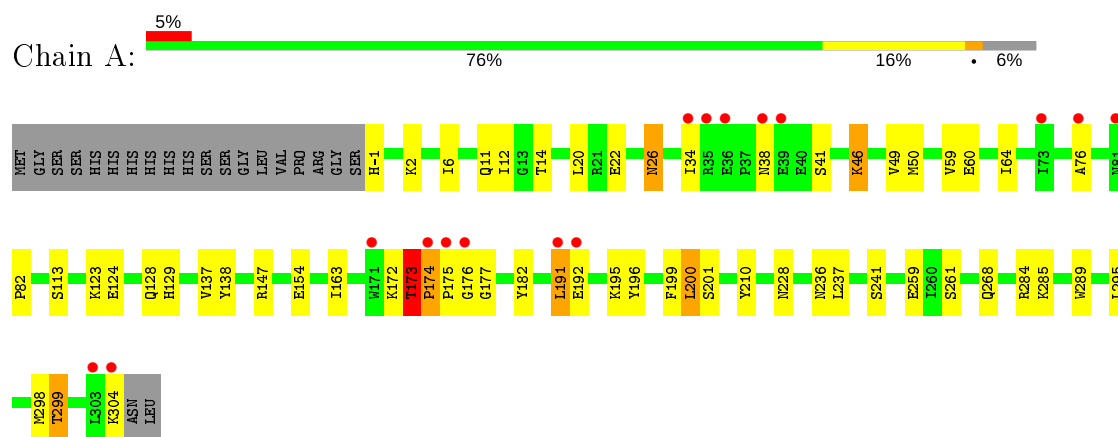
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	145	Total O 145 145	0	0
5	B	122	Total O 122 122	0	0
5	C	143	Total O 143 143	0	0
5	D	112	Total O 112 112	0	0

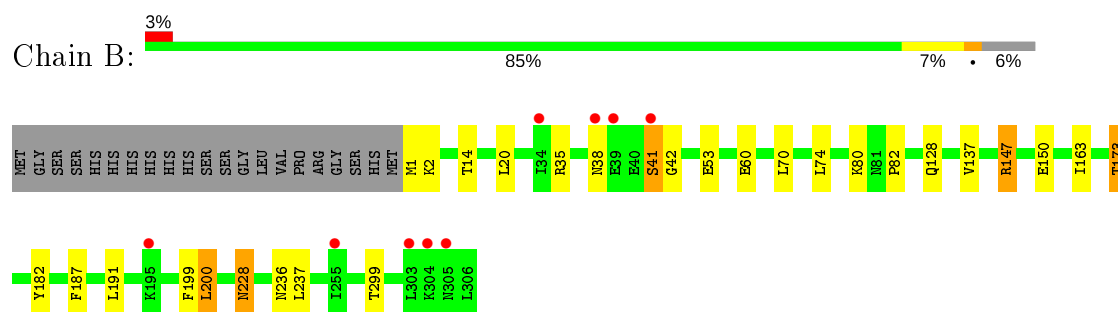
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

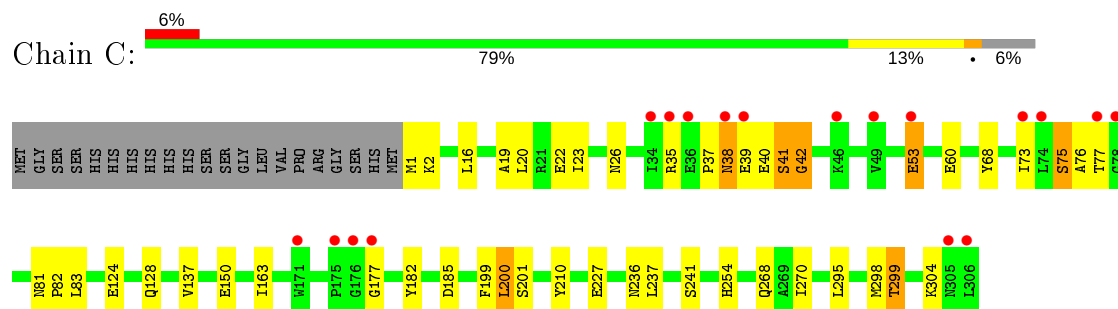
- Molecule 1: Artificial L-threonine 3-dehydrogenase



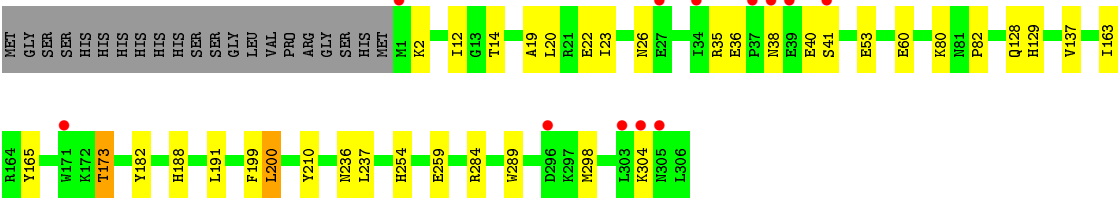
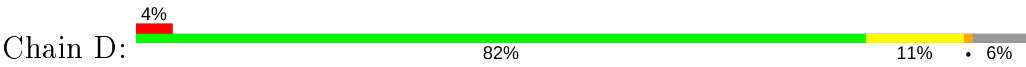
- Molecule 1: Artificial L-threonine 3-dehydrogenase



- Molecule 1: Artificial L-threonine 3-dehydrogenase



- Molecule 1: Artificial L-threonine 3-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.56 Å 112.69 Å 92.90 Å 90.00° 93.67° 90.00°	Depositor
Resolution (Å)	92.70 – 2.10 48.15 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (92.70-2.10) 99.8 (48.15-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.55 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.193 , 0.235 0.199 , 0.242	Depositor DCC
R_{free} test set	3612 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10523	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: PO4, 2PE, NAD

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	0.47	0/2499	0.63	3/3390 (0.1%)
1	B	0.46	0/2496	0.59	1/3387 (0.0%)
1	C	0.46	0/2496	0.60	0/3387
1	D	0.41	0/2496	0.54	0/3387
All	All	0.45	0/9987	0.59	4/13551 (0.0%)

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	1
1	C	0	3
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	A	147	ARG	NE-CZ-NH2	7.45	124.03	120.30
1	A	20	LEU	CB-CG-CD2	5.90	121.02	111.00
1	B	42	GLY	N-CA-C	-5.29	99.86	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	41	SER	Peptide
1	C	1	MET	Peptide
1	C	40	GLU	Peptide
1	C	75	SER	Peptide

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	2439	0	2380	53	0
1	B	2437	0	2381	14	0
1	C	2437	0	2381	29	0
1	D	2437	0	2381	20	0
2	A	44	0	26	8	0
2	B	44	0	26	1	0
2	D	44	0	26	2	0
3	A	10	0	0	0	0
3	B	10	0	0	1	0
3	C	5	0	0	1	0
3	D	10	0	0	0	0
4	B	28	0	38	1	0
4	C	28	0	38	2	0
4	D	28	0	38	3	0
5	A	145	0	0	3	0
5	B	122	0	0	0	0
5	C	143	0	0	2	0
5	D	112	0	0	4	0
All	All	10523	0	9715	114	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 (114) 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:174:PRO:HB2	1:A:175:PRO:HA	1.15	1.10
1:A:174:PRO:HB2	1:A:175:PRO:CA	1.84	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:SER:O	1:C:42:GLY:O	1.73	1.06
1:C:76:ALA:HB1	1:C:77:THR:HA	1.37	1.05
1:C:201:SER:H	1:C:268:GLN:HE22	1.16	0.93
1:A:201:SER:H	1:A:268:GLN:HE22	1.19	0.91
1:A:174:PRO:CB	1:A:175:PRO:HA	1.99	0.91
1:A:76:ALA:HB3	1:A:177:GLY:O	1.77	0.84
1:C:295:LEU:O	1:C:299:THR:HG23	1.80	0.81
1:B:147:ARG:HA	1:B:147:ARG:HE	1.45	0.80
1:A:138:TYR:HH	2:A:401:NAD:C2D	1.96	0.77
1:A:295:LEU:O	1:A:299:THR:HG23	1.83	0.77
1:C:150:GLU:OE1	3:C:402:PO4:O2	2.05	0.75
1:B:128:GLN:HE22	1:B:236:ASN:H	1.32	0.75
1:C:128:GLN:HE22	1:C:236:ASN:H	1.35	0.74
1:A:14:THR:OG1	1:A:172:LYS:HE3	1.88	0.73
1:A:113:SER:HB2	2:A:401:NAD:H6N	1.72	0.70
1:A:128:GLN:HE22	1:A:236:ASN:H	1.40	0.70
1:A:284:ARG:HG2	1:A:289:TRP:O	1.94	0.68
1:B:147:ARG:NH2	1:B:150:GLU:OE1	2.26	0.68
1:A:138:TYR:OH	2:A:401:NAD:O2D	1.58	0.68
1:D:128:GLN:HE22	1:D:236:ASN:H	1.42	0.67
1:B:14:THR:HG21	1:B:173:THR:HG21	1.75	0.67
1:D:40:GLU:O	1:D:41:SER:OG	2.12	0.67
1:A:6:ILE:CG2	1:A:49:VAL:HG11	2.25	0.67
1:D:14:THR:HG21	1:D:173:THR:HG21	1.76	0.66
1:D:129:HIS:HE1	5:D:603:HOH:O	1.78	0.65
1:A:201:SER:H	1:A:268:GLN:NE2	1.90	0.65
1:A:26:ASN:OD1	1:A:41:SER:O	2.14	0.65
1:C:201:SER:H	1:C:268:GLN:NE2	1.89	0.65
1:A:173:THR:CB	1:A:174:PRO:HA	2.28	0.64
1:D:254:HIS:HE1	5:D:584:HOH:O	1.81	0.64
1:A:174:PRO:CB	1:A:175:PRO:CA	2.65	0.64
1:C:82:PRO:HB3	1:C:137:VAL:HG21	1.80	0.63
1:C:75:SER:HB2	5:C:544:HOH:O	1.99	0.63
1:A:138:TYR:CZ	2:A:401:NAD:O2D	2.35	0.62
1:A:173:THR:HB	1:A:174:PRO:HA	1.82	0.62
1:D:284:ARG:HG2	1:D:289:TRP:O	1.99	0.61
1:C:76:ALA:CB	1:C:77:THR:HA	2.15	0.61
1:D:188:HIS:HD2	5:D:516:HOH:O	1.84	0.61
1:A:138:TYR:CE1	2:A:401:NAD:O2D	2.54	0.61
1:A:173:THR:HB	1:A:174:PRO:CA	2.31	0.60
1:A:191:LEU:CD1	1:A:191:LEU:C	2.71	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PRO:HD2	1:A:177:GLY:HA2	1.85	0.58
1:C:75:SER:HA	4:C:401:2PE:H152	1.86	0.57
1:A:129:HIS:HE1	5:A:625:HOH:O	1.86	0.57
1:A:138:TYR:OH	2:A:401:NAD:C2D	2.49	0.57
1:A:191:LEU:C	1:A:191:LEU:HD12	2.25	0.57
1:D:82:PRO:HB3	1:D:137:VAL:HG21	1.87	0.56
1:A:59:VAL:HG13	1:A:64:ILE:HB	1.88	0.56
1:A:163:ILE:HG21	1:A:237:LEU:HD22	1.89	0.55
1:B:128:GLN:NE2	1:B:236:ASN:H	2.03	0.55
1:D:129:HIS:HD2	5:D:527:HOH:O	1.90	0.55
1:C:163:ILE:HG21	1:C:237:LEU:HD22	1.89	0.55
1:C:19:ALA:O	1:C:23:ILE:HG22	2.08	0.55
1:D:80:LYS:HZ2	4:D:402:2PE:H261	1.71	0.55
1:A:195:LYS:NZ	1:A:261:SER:OG	2.35	0.54
1:A:82:PRO:HB3	1:A:137:VAL:HG21	1.88	0.54
1:D:80:LYS:NZ	4:D:402:2PE:H261	2.22	0.54
1:A:173:THR:HG22	1:A:174:PRO:HA	1.90	0.54
1:D:80:LYS:HE2	4:D:402:2PE:H172	1.89	0.54
1:D:163:ILE:HG21	1:D:237:LEU:HD22	1.90	0.53
1:A:195:LYS:HG3	1:A:196:TYR:N	2.23	0.53
1:B:163:ILE:HG21	1:B:237:LEU:HD22	1.91	0.53
1:C:37:PRO:O	1:C:38:ASN:HB2	2.07	0.53
1:A:34:ILE:O	1:A:46:LYS:HD2	2.09	0.53
1:B:82:PRO:HB3	1:B:137:VAL:HG21	1.90	0.53
1:D:19:ALA:O	1:D:23:ILE:HG22	2.08	0.53
1:A:6:ILE:CG2	1:A:49:VAL:CG1	2.87	0.53
1:D:53:GLU:OE1	1:D:53:GLU:HA	2.09	0.53
1:B:147:ARG:HA	1:B:147:ARG:NE	2.20	0.52
1:C:270:ILE:HD13	4:C:401:2PE:H121	1.91	0.51
1:C:199:PHE:HD1	1:C:200:LEU:HD13	1.75	0.51
1:A:173:THR:CG2	1:A:174:PRO:HA	2.42	0.49
1:C:199:PHE:CD1	1:C:200:LEU:HD13	2.47	0.49
1:A:176:GLY:N	1:A:177:GLY:CA	2.76	0.49
1:A:11:GLN:HB2	1:A:174:PRO:HD2	1.95	0.48
1:A:285:LYS:HD3	1:A:285:LYS:C	2.34	0.48
1:C:254:HIS:HE1	5:C:527:HOH:O	1.97	0.47
1:A:49:VAL:HG13	2:A:401:NAD:C2A	2.44	0.47
1:A:210:TYR:CD2	1:A:298:MET:HG3	2.50	0.47
1:B:80:LYS:HE2	4:B:402:2PE:H112	1.96	0.47
1:A:123:LYS:NZ	5:A:501:HOH:O	2.48	0.46
1:A:173:THR:CB	1:A:174:PRO:CA	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:TYR:CD2	1:D:298:MET:HG3	2.51	0.46
1:C:73:ILE:HG22	1:C:75:SER:H	1.81	0.46
1:A:201:SER:N	1:A:268:GLN:HE22	2.00	0.46
1:C:37:PRO:O	1:C:38:ASN:CB	2.63	0.46
1:A:195:LYS:CG	1:A:196:TYR:N	2.79	0.46
1:A:199:PHE:CD1	1:A:200:LEU:HD13	2.51	0.46
1:D:199:PHE:CD1	1:D:200:LEU:HD13	2.50	0.45
1:A:174:PRO:HB2	1:A:175:PRO:CB	2.44	0.45
1:A:14:THR:HG1	1:A:172:LYS:HE3	1.81	0.45
1:D:165:TYR:HB2	2:D:401:NAD:C5N	2.47	0.45
1:C:41:SER:C	1:C:42:GLY:O	2.44	0.44
1:B:199:PHE:CD1	1:B:200:LEU:HD13	2.52	0.44
1:A:12:ILE:HD12	2:A:401:NAD:H51N	1.99	0.44
1:C:81:ASN:HB3	1:C:83:LEU:H	1.83	0.44
1:D:12:ILE:HD12	2:D:401:NAD:H51N	1.99	0.44
1:A:124:GLU:HG3	1:C:241:SER:HB3	2.00	0.43
1:C:128:GLN:NE2	1:C:236:ASN:H	2.10	0.43
1:A:6:ILE:HG21	1:A:49:VAL:HG11	1.97	0.43
1:C:16:LEU:HD21	1:C:68:TYR:CD1	2.54	0.43
1:C:210:TYR:CD2	1:C:298:MET:HG3	2.54	0.43
1:A:241:SER:HB3	1:C:124:GLU:HG3	2.00	0.42
1:C:81:ASN:HA	1:C:82:PRO:HD3	1.89	0.42
1:B:70:LEU:O	2:B:401:NAD:H52N	2.20	0.42
1:B:150:GLU:OE1	3:B:404:PO4:O4	2.38	0.42
1:B:187:PHE:HE1	1:B:299:THR:HG23	1.86	0.41
1:B:228:ASN:N	1:B:228:ASN:HD22	2.18	0.41
1:D:199:PHE:HD1	1:D:200:LEU:HD13	1.84	0.41
1:A:172:LYS:HB3	5:A:502:HOH:O	2.19	0.41
1:A:191:LEU:HD12	1:A:192:GLU:N	2.36	0.40
1:C:53:GLU:HG3	1:C:53:GLU:H	1.68	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	304/327 (93%)	291 (96%)	11 (4%)	2 (1%)	22	18
1	B	304/327 (93%)	295 (97%)	9 (3%)	0	100	100
1	C	304/327 (93%)	291 (96%)	9 (3%)	4 (1%)	12	7
1	D	304/327 (93%)	295 (97%)	9 (3%)	0	100	100
All	All	1216/1308 (93%)	1172 (96%)	38 (3%)	6 (0%)	29	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	PRO
1	C	38	ASN
1	C	42	GLY
1	C	39	GLU
1	A	173	THR
1	C	177	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	265/283 (94%)	248 (94%)	17 (6%)	17	14
1	B	265/283 (94%)	250 (94%)	15 (6%)	20	18
1	C	265/283 (94%)	251 (95%)	14 (5%)	22	20
1	D	265/283 (94%)	251 (95%)	14 (5%)	22	20
All	All	1060/1132 (94%)	1000 (94%)	60 (6%)	20	18

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	2	LYS

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Mol	Chain	Res	Type
1	A	22	GLU
1	A	26	ASN
1	A	38	ASN
1	A	46	LYS
1	A	50	MET
1	A	60	GLU
1	A	154	GLU
1	A	173	THR
1	A	182	TYR
1	A	191	LEU
1	A	200	LEU
1	A	228	ASN
1	A	259	GLU
1	A	299	THR
1	A	304	LYS
1	B	1	MET
1	B	2	LYS
1	B	20	LEU
1	B	35	ARG
1	B	38	ASN
1	B	41	SER
1	B	53	GLU
1	B	60	GLU
1	B	74	LEU
1	B	147	ARG
1	B	173	THR
1	B	182	TYR
1	B	191	LEU
1	B	200	LEU
1	B	228	ASN
1	C	2	LYS
1	C	20	LEU
1	C	22	GLU
1	C	26	ASN
1	C	35	ARG
1	C	41	SER
1	C	53	GLU
1	C	60	GLU
1	C	182	TYR
1	C	185	ASP
1	C	200	LEU
1	C	227	GLU

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Mol	Chain	Res	Type
1	C	299	THR
1	C	304	LYS
1	D	2	LYS
1	D	20	LEU
1	D	22	GLU
1	D	26	ASN
1	D	35	ARG
1	D	36	GLU
1	D	38	ASN
1	D	60	GLU
1	D	173	THR
1	D	182	TYR
1	D	191	LEU
1	D	200	LEU
1	D	259	GLU
1	D	304	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	91	ASN
1	A	128	GLN
1	A	129	HIS
1	A	228	ASN
1	A	254	HIS
1	A	268	GLN
1	B	28	ASN
1	B	91	ASN
1	B	128	GLN
1	B	228	ASN
1	C	28	ASN
1	C	69	HIS
1	C	125	ASN
1	C	128	GLN
1	C	254	HIS
1	C	268	GLN
1	D	28	ASN
1	D	91	ASN
1	D	128	GLN
1	D	129	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 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	NAD	B	401	-	42,48,48	1.00	3 (7%)	50,73,73	1.29	6 (12%)
2	NAD	D	401	-	42,48,48	0.87	2 (4%)	50,73,73	1.26	5 (10%)
3	PO4	A	402	-	4,4,4	0.63	0	6,6,6	0.76	0
3	PO4	D	404	-	4,4,4	0.89	0	6,6,6	0.74	0
2	NAD	A	401	-	42,48,48	0.96	2 (4%)	50,73,73	1.33	7 (14%)
3	PO4	C	402	-	4,4,4	1.12	0	6,6,6	0.48	0
3	PO4	B	404	-	4,4,4	1.08	0	6,6,6	0.74	0
4	2PE	D	402	-	27,27,27	0.54	0	26,26,26	0.30	0
3	PO4	A	403	-	4,4,4	1.24	0	6,6,6	0.40	0
3	PO4	D	403	-	4,4,4	0.63	0	6,6,6	0.96	0
3	PO4	B	403	-	4,4,4	0.80	0	6,6,6	1.15	1 (16%)
4	2PE	B	402	-	27,27,27	0.56	0	26,26,26	0.28	0
4	2PE	C	401	-	27,27,27	0.60	0	26,26,26	0.53	0

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	NAD	B	401	-	-	2/26/62/62	0/5/5/5
2	NAD	D	401	-	-	4/26/62/62	0/5/5/5
2	NAD	A	401	-	-	2/26/62/62	0/5/5/5
4	2PE	D	402	-	-	10/25/25/25	-
4	2PE	B	402	-	-	16/25/25/25	-
4	2PE	C	401	-	-	14/25/25/25	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAD	O4D-C1D	3.30	1.45	1.41
2	A	401	NAD	O4D-C1D	3.11	1.45	1.41
2	B	401	NAD	C5A-C4A	2.57	1.47	1.40
2	D	401	NAD	O4D-C1D	2.55	1.44	1.41
2	A	401	NAD	C5A-C4A	2.47	1.47	1.40
2	D	401	NAD	C5A-C4A	2.34	1.47	1.40
2	B	401	NAD	C2A-N3A	2.20	1.35	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAD	N3A-C2A-N1A	-4.16	122.18	128.68
2	A	401	NAD	N3A-C2A-N1A	-3.78	122.77	128.68
2	B	401	NAD	N3A-C2A-N1A	-3.75	122.82	128.68
2	A	401	NAD	C4A-C5A-N7A	-3.48	105.77	109.40
2	B	401	NAD	C4A-C5A-N7A	-3.47	105.78	109.40
2	D	401	NAD	C1B-N9A-C4A	-2.99	121.39	126.64
2	D	401	NAD	PN-O3-PA	-2.93	122.77	132.83
2	D	401	NAD	C4A-C5A-N7A	-2.92	106.36	109.40
2	B	401	NAD	C1B-N9A-C4A	-2.77	121.78	126.64
2	B	401	NAD	PN-O3-PA	-2.66	123.69	132.83
2	D	401	NAD	C2A-N1A-C6A	2.60	123.20	118.75
2	A	401	NAD	C6N-N1N-C2N	-2.54	119.65	121.97
2	A	401	NAD	C1B-N9A-C4A	-2.49	122.27	126.64
2	A	401	NAD	PN-O3-PA	-2.28	124.99	132.83
2	A	401	NAD	C2A-N1A-C6A	2.25	122.60	118.75
2	B	401	NAD	O2A-PA-O1A	2.17	122.97	112.24
3	B	403	PO4	O4-P-O1	-2.10	103.20	110.89
2	B	401	NAD	C2A-N1A-C6A	2.09	122.34	118.75
2	A	401	NAD	C3N-C7N-N7N	2.05	120.21	117.75

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	NAD	C5D-O5D-PN-O2N
4	C	401	2PE	C14-C15-O16-C17
4	D	402	2PE	O22-C23-C24-O25
4	C	401	2PE	O16-C17-C18-O19
4	B	402	2PE	O4-C5-C6-O7
4	B	402	2PE	O22-C23-C24-O25
4	C	401	2PE	O22-C23-C24-O25
4	B	402	2PE	O1-C2-C3-O4
4	D	402	2PE	O10-C11-C12-O13
4	B	402	2PE	O19-C20-C21-O22
4	C	401	2PE	O25-C26-C27-O28
4	D	402	2PE	O4-C5-C6-O7
4	B	402	2PE	O13-C14-C15-O16
4	C	401	2PE	O7-C8-C9-O10
4	B	402	2PE	O25-C26-C27-O28
4	B	402	2PE	O10-C11-C12-O13
4	D	402	2PE	C2-C3-O4-C5
4	B	402	2PE	C24-C23-O22-C21
4	D	402	2PE	C24-C23-O22-C21
4	D	402	2PE	C9-C8-O7-C6
4	B	402	2PE	C20-C21-O22-C23
4	B	402	2PE	C12-C11-O10-C9
4	C	401	2PE	C5-C6-O7-C8
4	D	402	2PE	C18-C17-O16-C15
2	D	401	NAD	C5D-O5D-PN-O3
4	D	402	2PE	O16-C17-C18-O19
4	B	402	2PE	C17-C18-O19-C20
2	D	401	NAD	C5D-O5D-PN-O1N
4	D	402	2PE	O13-C14-C15-O16
4	B	402	2PE	C9-C8-O7-C6
4	B	402	2PE	C8-C9-O10-C11
4	B	402	2PE	C23-C24-O25-C26
4	D	402	2PE	O19-C20-C21-O22
4	C	401	2PE	C6-C5-O4-C3
4	C	401	2PE	C23-C24-O25-C26
4	C	401	2PE	O4-C5-C6-O7
4	C	401	2PE	O19-C20-C21-O22
4	C	401	2PE	C21-C20-O19-C18
2	A	401	NAD	O4B-C4B-C5B-O5B
4	C	401	2PE	C12-C11-O10-C9

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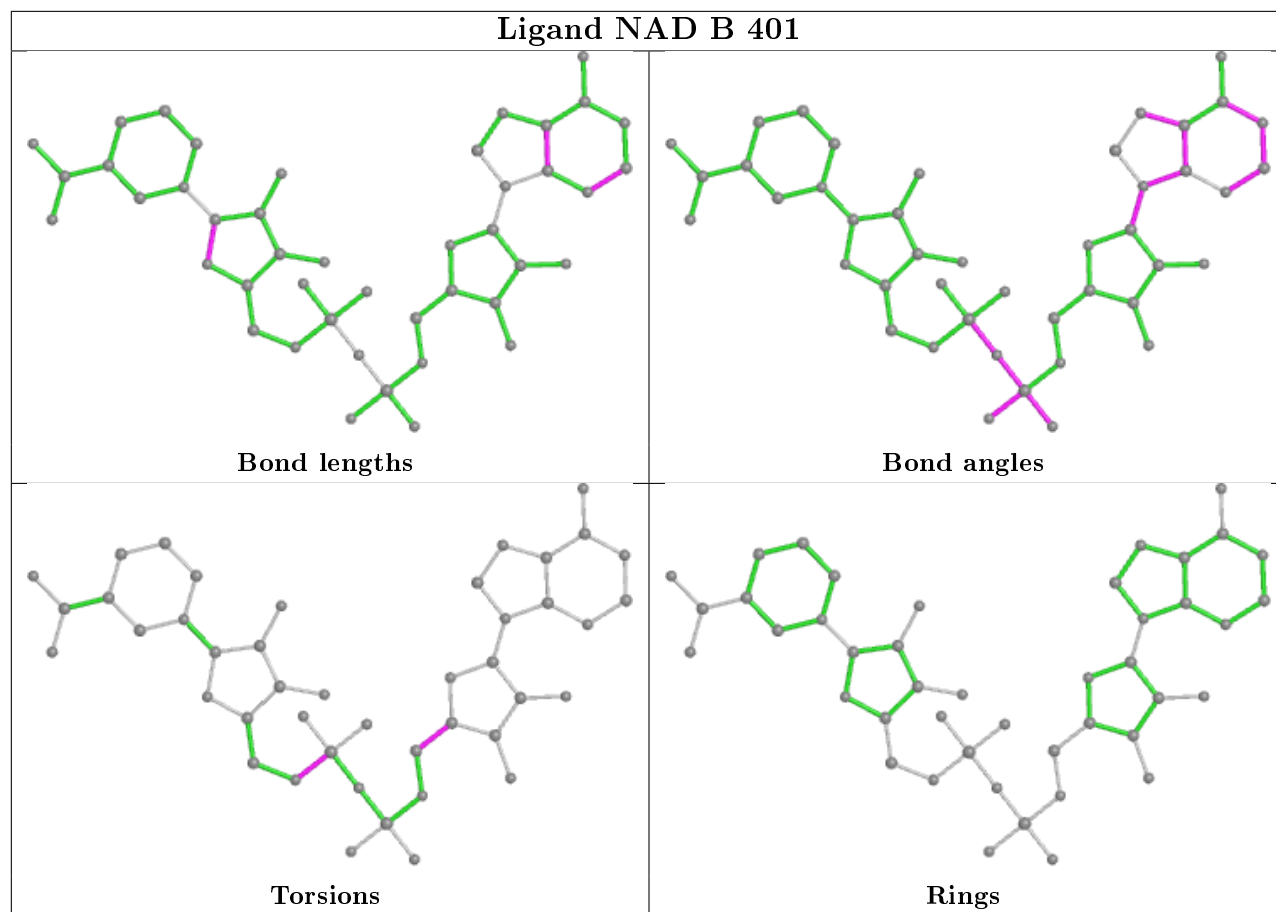
Mol	Chain	Res	Type	Atoms
4	B	402	2PE	O7-C8-C9-O10
4	C	401	2PE	C18-C17-O16-C15
2	B	401	NAD	C5D-O5D-PN-O3
2	A	401	NAD	C5D-O5D-PN-O3
4	B	402	2PE	C6-C5-O4-C3
2	D	401	NAD	O4B-C4B-C5B-O5B
4	C	401	2PE	O13-C14-C15-O16
2	B	401	NAD	O4B-C4B-C5B-O5B

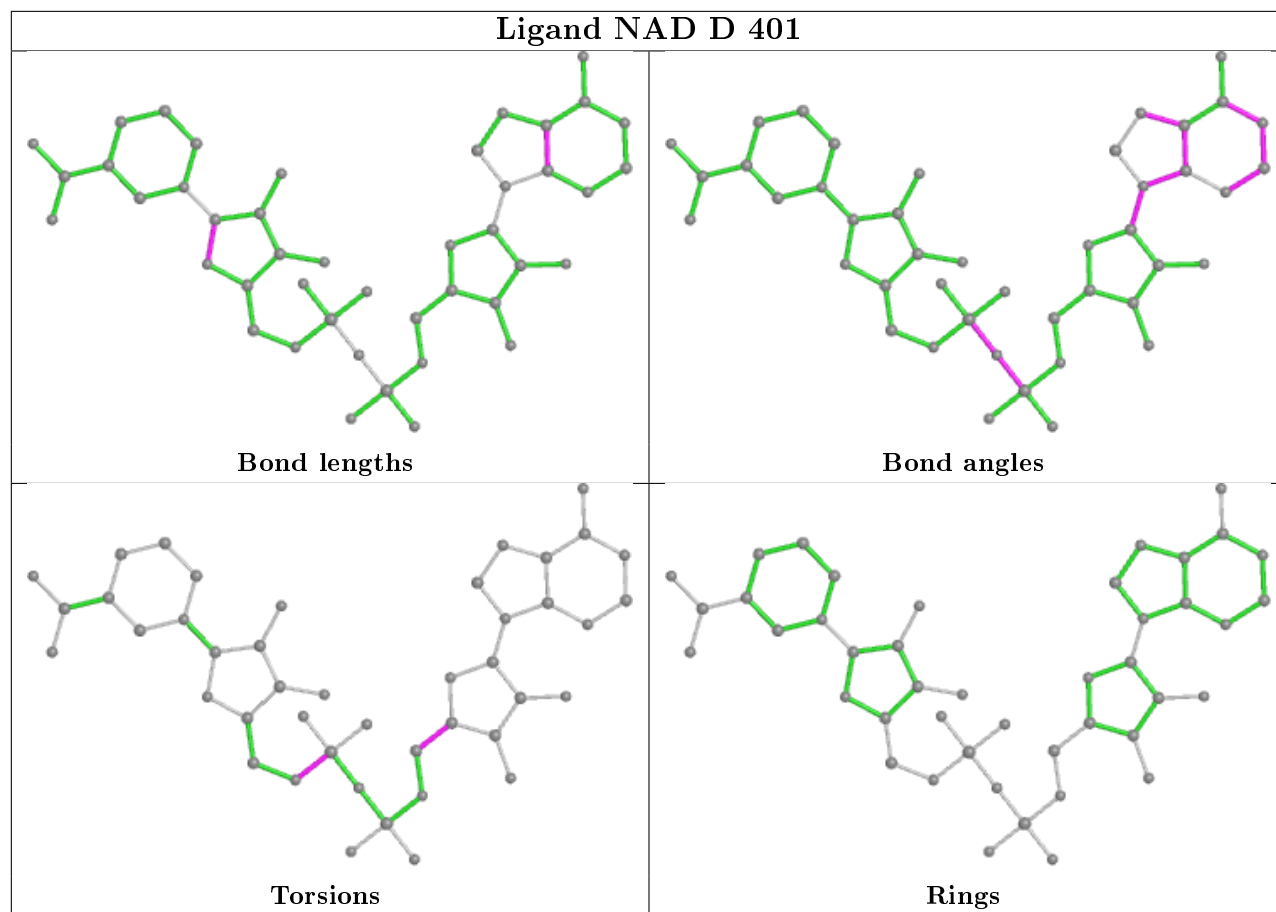
There are no ring outliers.

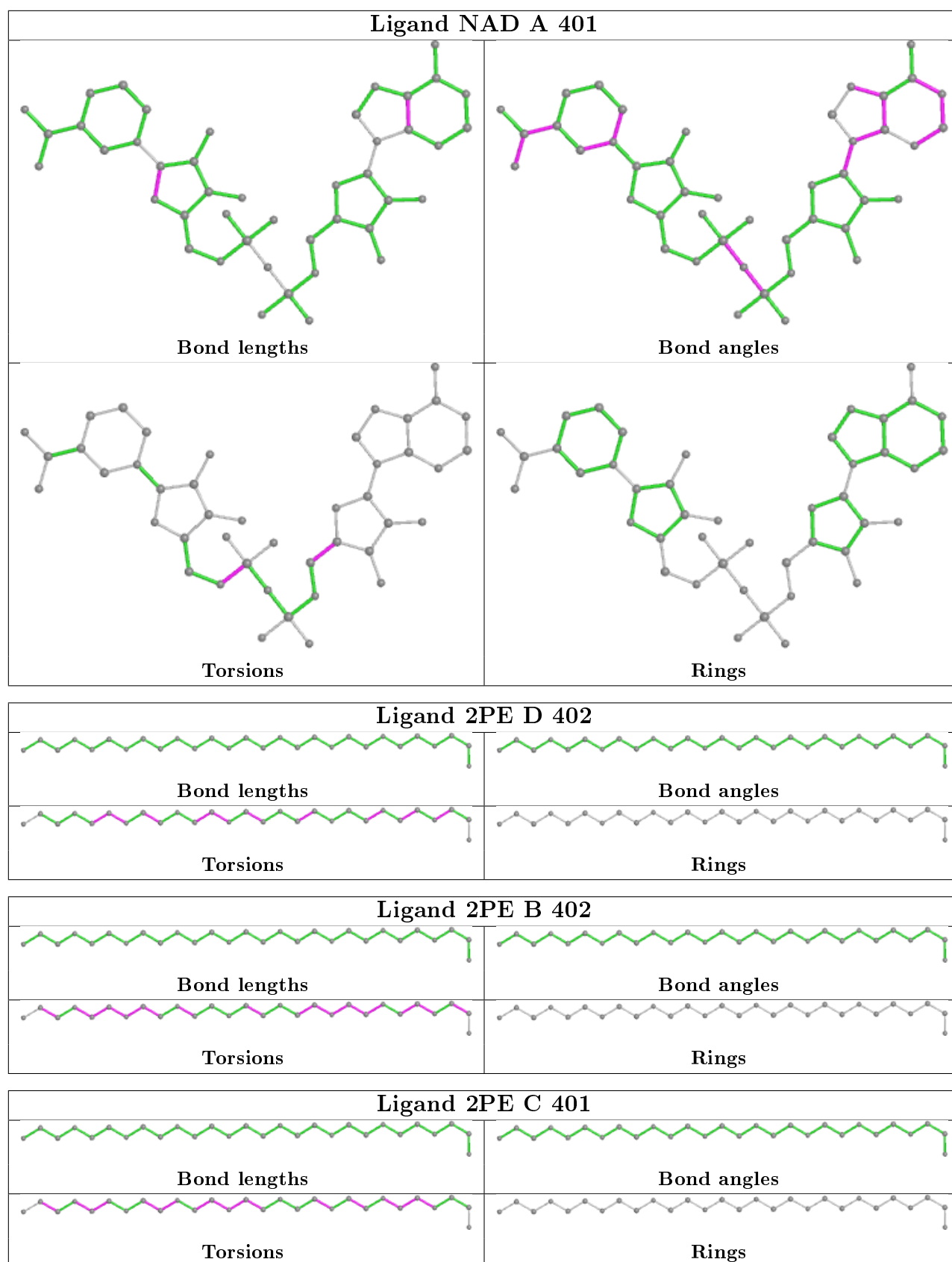
8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NAD	1	0
2	D	401	NAD	2	0
2	A	401	NAD	8	0
3	C	402	PO4	1	0
3	B	404	PO4	1	0
4	D	402	2PE	3	0
4	B	402	2PE	1	0
4	C	401	2PE	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

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 ⓘ

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	306/327 (93%)	0.11	16 (5%) 27 32	14, 29, 68, 106	0
1	B	306/327 (93%)	0.08	9 (2%) 51 57	16, 28, 56, 88	0
1	C	306/327 (93%)	0.28	18 (5%) 22 27	16, 33, 76, 146	0
1	D	306/327 (93%)	0.18	12 (3%) 39 45	18, 34, 65, 119	0
All	All	1224/1308 (93%)	0.16	55 (4%) 33 38	14, 31, 67, 146	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	GLY	6.7
1	A	175	PRO	5.9
1	D	38	ASN	5.7
1	D	1	MET	5.5
1	C	77	THR	5.3
1	C	78	GLY	4.7
1	C	38	ASN	4.6
1	A	174	PRO	4.4
1	C	306	LEU	4.3
1	C	171	TRP	4.0
1	D	39	GLU	4.0
1	C	74	LEU	3.8
1	D	171	TRP	3.7
1	C	39	GLU	3.7
1	A	38	ASN	3.6
1	C	35	ARG	3.6
1	D	41	SER	3.5
1	D	305	ASN	3.4
1	A	35	ARG	3.3
1	A	191	LEU	3.2
1	C	177	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	36	GLU	3.1
1	D	27	GLU	3.1
1	A	76	ALA	3.0
1	D	303	LEU	2.9
1	A	192	GLU	2.8
1	C	305	ASN	2.8
1	D	304	LYS	2.7
1	A	34	ILE	2.7
1	B	38	ASN	2.7
1	C	73	ILE	2.6
1	C	176	GLY	2.5
1	A	303	LEU	2.5
1	B	303	LEU	2.5
1	C	53	GLU	2.5
1	C	49	VAL	2.4
1	B	305	ASN	2.4
1	C	175	PRO	2.4
1	A	171	TRP	2.4
1	B	195	LYS	2.3
1	A	73	ILE	2.3
1	D	34	ILE	2.3
1	A	304	LYS	2.3
1	A	36	GLU	2.2
1	D	296	ASP	2.2
1	D	37	PRO	2.1
1	A	81	ASN	2.1
1	B	41	SER	2.1
1	C	46	LYS	2.1
1	B	34	ILE	2.1
1	B	255	ILE	2.1
1	A	39	GLU	2.0
1	B	39	GLU	2.0
1	B	304	LYS	2.0
1	C	34	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

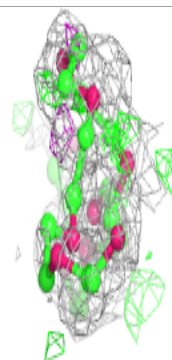
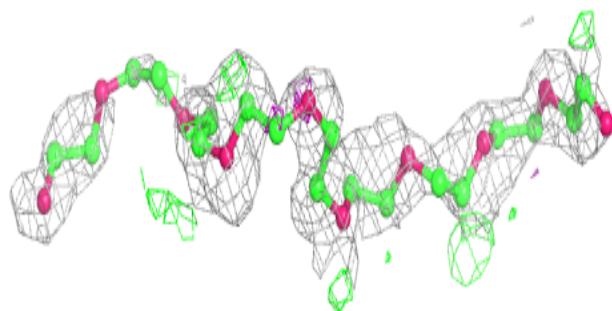
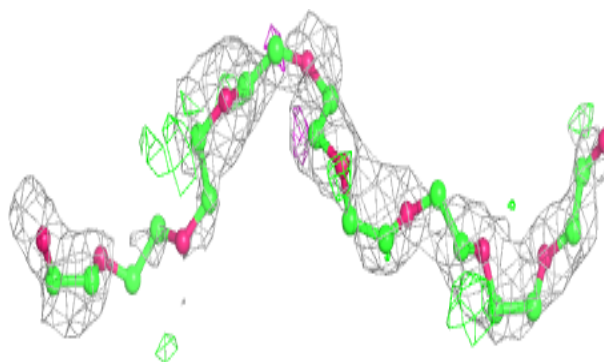
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	2PE	C	401	28/28	0.71	0.27	41,59,77,81	0
4	2PE	D	402	28/28	0.77	0.20	53,66,96,101	0
4	2PE	B	402	28/28	0.81	0.22	46,57,80,82	0
2	NAD	A	401	44/44	0.81	0.33	31,63,85,90	0
3	PO4	C	402	5/5	0.87	0.24	26,29,35,36	5
3	PO4	A	403	5/5	0.87	0.33	25,30,33,38	5
3	PO4	B	404	5/5	0.90	0.32	25,29,29,34	5
2	NAD	B	401	44/44	0.92	0.19	27,36,43,48	0
2	NAD	D	401	44/44	0.93	0.19	31,42,50,56	0
3	PO4	A	402	5/5	0.94	0.14	45,56,62,62	0
3	PO4	D	403	5/5	0.95	0.10	39,43,46,46	0
3	PO4	D	404	5/5	0.97	0.10	38,39,43,46	0
3	PO4	B	403	5/5	0.97	0.10	37,37,43,44	0

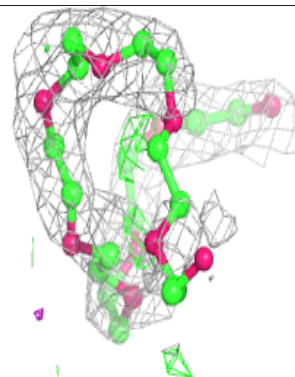
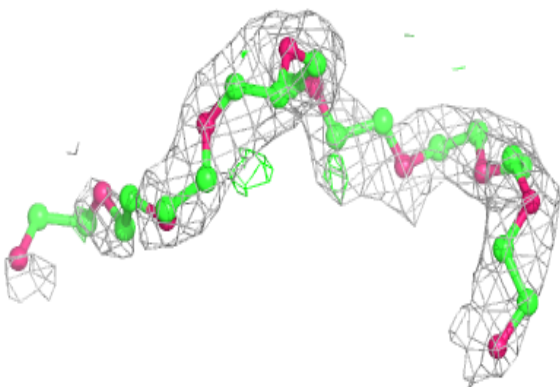
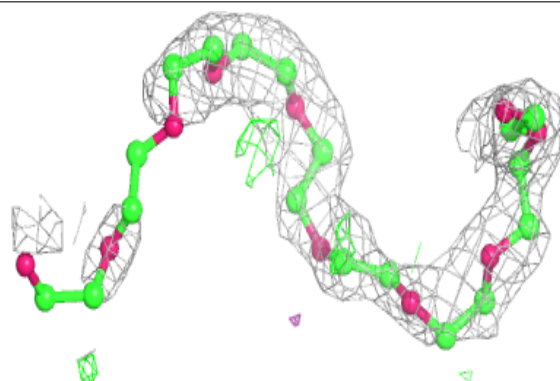
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2PE C 401:

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

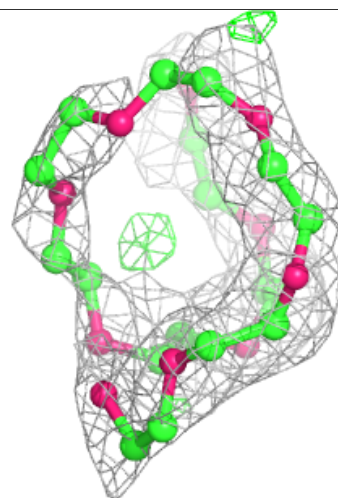
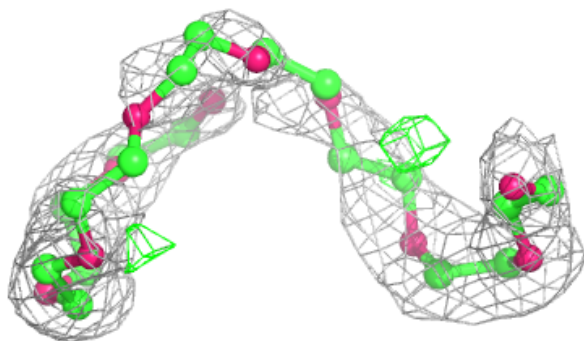
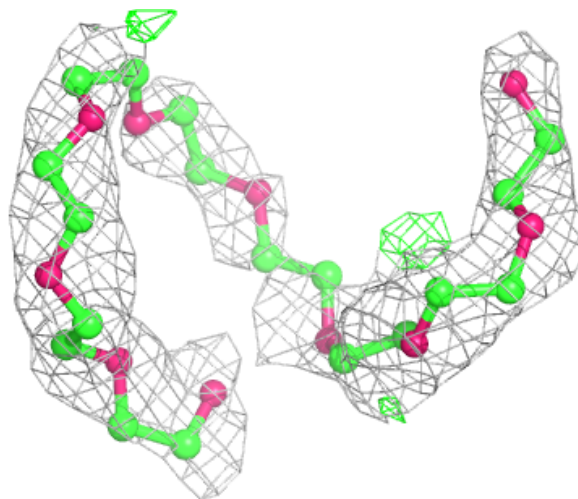
**Electron density around 2PE D 402:**

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



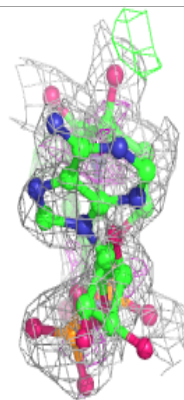
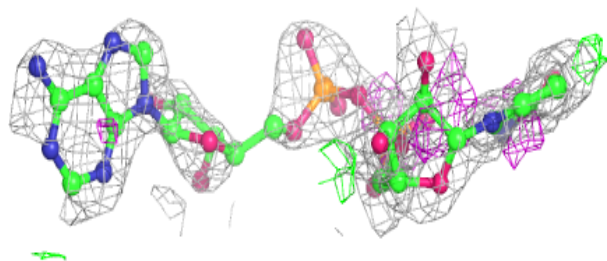
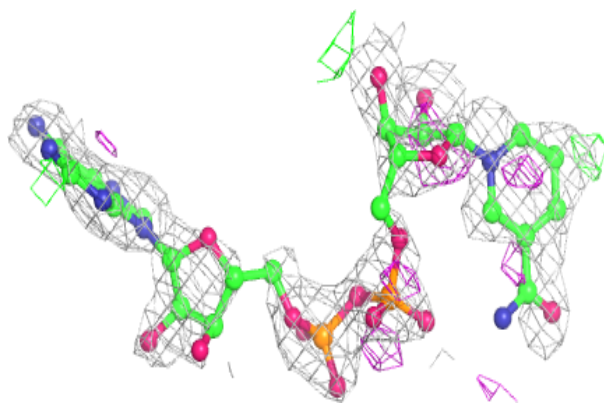
Electron density around 2PE B 402:

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

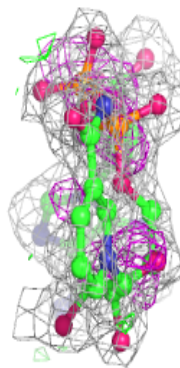
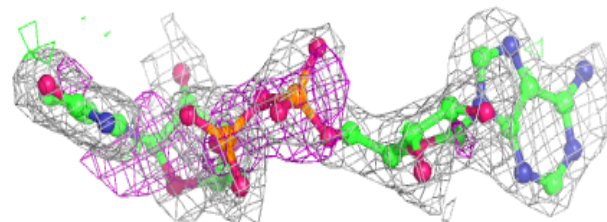
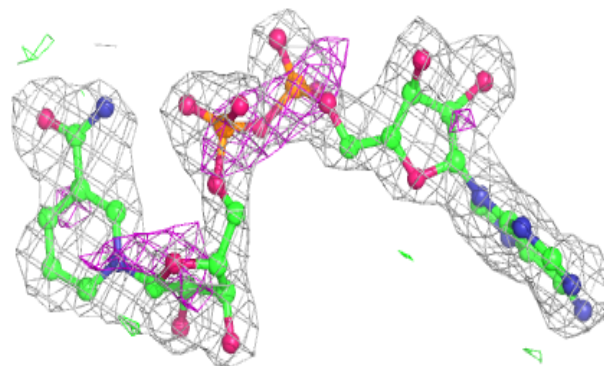


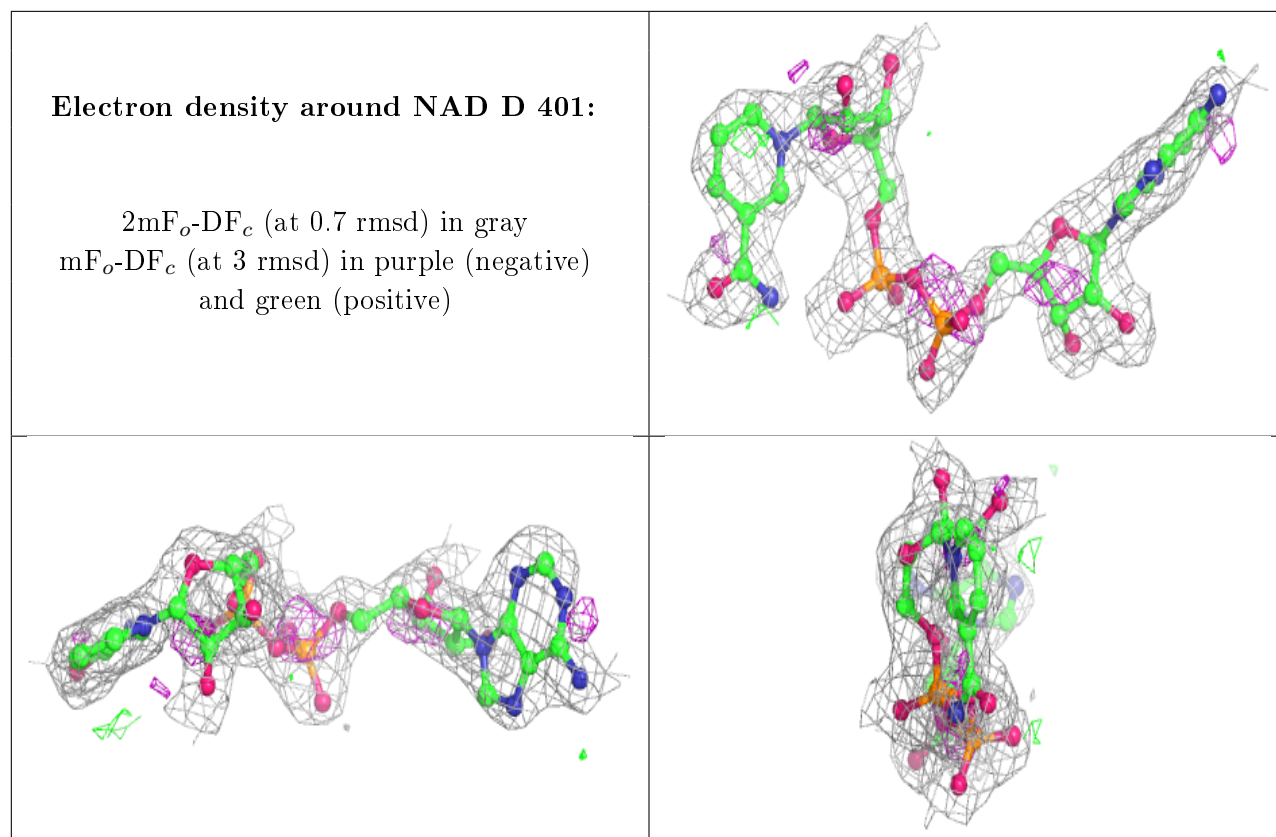
Electron density around NAD A 401:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.