



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:00 PM UTC

PDB ID : 1LI4 / pdb_00001li4
Title : Human S-adenosylhomocysteine hydrolase complexed with neplanocin
Authors : Yang, X.; Hu, Y.; Yin, D.H.; Turner, M.A.; Wang, M.; Borchardt, R.T.;
Howell, P.L.; Kuczera, K.; Schowen, R.L.
Deposited on : 2002-04-17
Resolution : 2.01 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

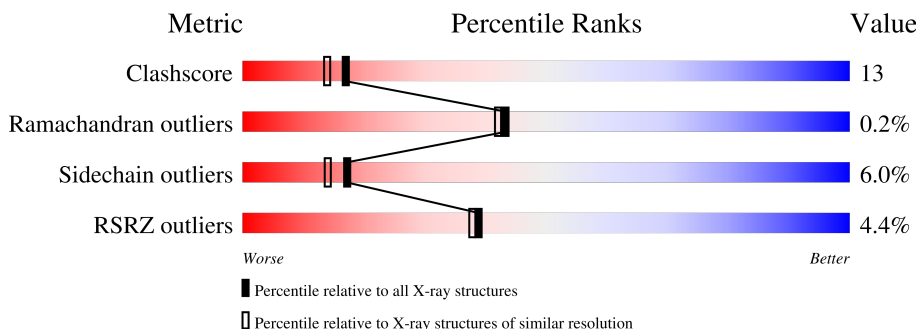
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



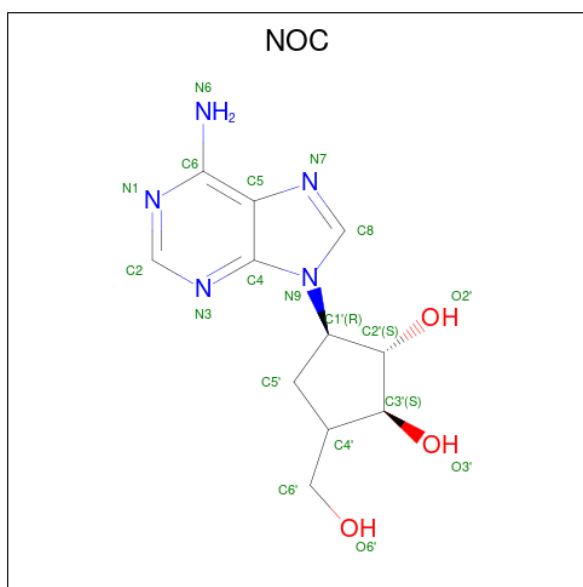
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	432	4% 69% 25% 5%

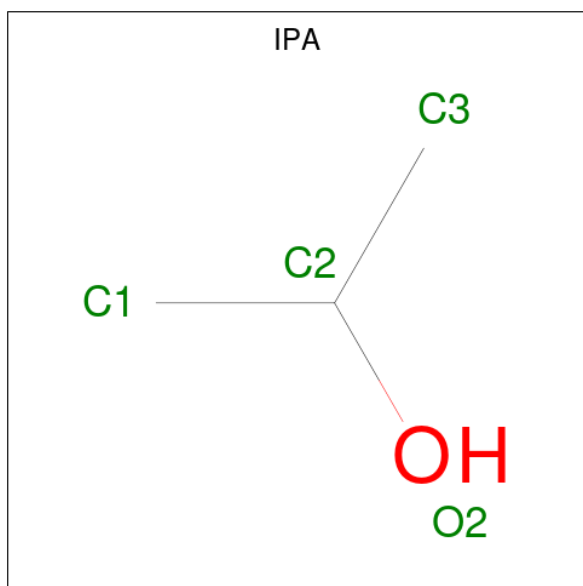
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NOC	A	434	X	-	-	-



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	11	5	3		

- Molecule 4 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	3	1		
4	A	1	Total	C	O	0	0
			4	3	1		

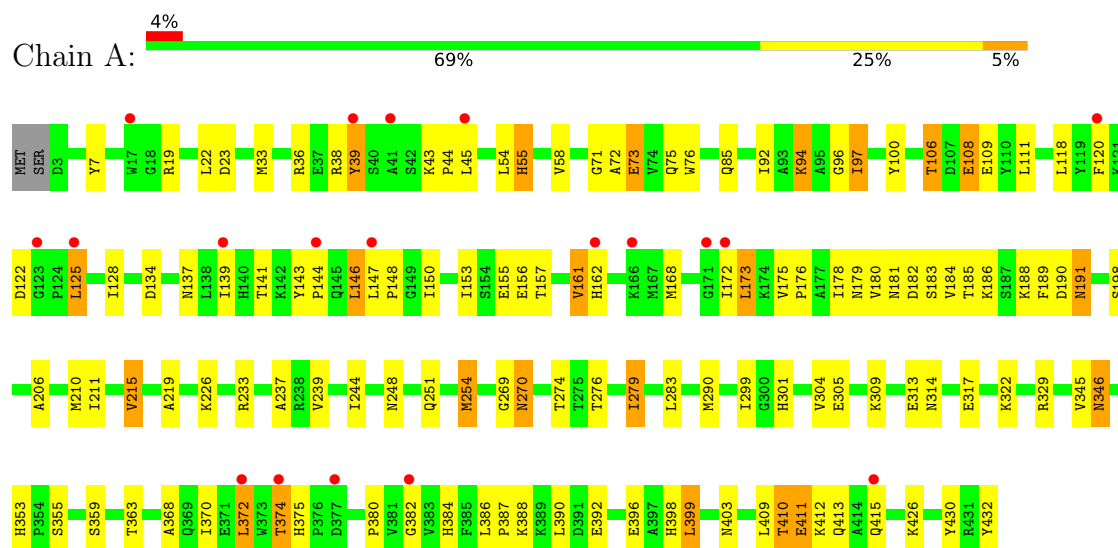
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	213	Total 213	O 213	0	0

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: S-adenosylhomocysteine hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.83Å 135.67Å 171.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.71 – 2.01 29.71 – 2.01	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.71-2.01) 95.2 (29.71-2.01)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.236 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.0	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	3606	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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, IPA, NOC

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	0.98	3/3386 (0.1%)	1.19	31/4585 (0.7%)

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	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	MET	SD-CE	-6.96	1.62	1.79
1	A	290	MET	SD-CE	-6.92	1.62	1.79
1	A	219	ALA	CA-CB	5.55	1.60	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	GLU	N-CA-C	8.96	121.13	111.36
1	A	279	ILE	CB-CA-C	-8.60	102.13	111.59
1	A	276	THR	N-CA-C	7.28	121.40	112.23
1	A	183	SER	N-CA-C	-7.14	100.44	110.50
1	A	299	ILE	N-CA-C	-7.04	106.44	113.20
1	A	239	VAL	N-CA-C	6.91	118.07	107.99
1	A	106	THR	N-CA-C	-6.85	100.66	110.59
1	A	290	MET	N-CA-C	6.83	120.39	110.28
1	A	386	LEU	N-CA-C	-6.66	100.90	110.08
1	A	301	HIS	N-CA-C	6.65	119.13	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	GLY	N-CA-C	6.64	119.12	111.36
1	A	270	ASN	N-CA-C	-6.54	105.59	113.97
1	A	43	LYS	CB-CA-C	-6.54	106.56	111.20
1	A	157	THR	N-CA-C	6.48	120.08	109.85
1	A	71	GLY	N-CA-C	6.45	123.30	114.92
1	A	363	THR	N-CA-C	-6.42	104.36	111.36
1	A	76	TRP	N-CA-C	6.23	119.34	109.50
1	A	345	VAL	N-CA-C	6.07	118.67	111.09
1	A	410	THR	N-CA-C	-6.00	102.45	110.55
1	A	215	VAL	N-CA-C	-5.85	99.99	108.36
1	A	73	GLU	N-CA-C	-5.85	100.17	109.76
1	A	39	TYR	N-CA-C	5.82	121.09	113.30
1	A	182	ASP	N-CA-C	5.81	120.06	113.15
1	A	172	ILE	CB-CA-C	-5.71	104.59	112.24
1	A	97	ILE	CA-C-N	-5.65	113.45	120.79
1	A	97	ILE	C-N-CA	-5.65	113.45	120.79
1	A	314	ASN	N-CA-C	5.43	120.78	113.72
1	A	122	ASP	N-CA-C	5.40	118.95	111.55
1	A	244	ILE	N-CA-C	-5.24	107.30	113.42
1	A	153	ILE	CB-CA-C	-5.22	102.71	110.33
1	A	355	SER	N-CA-C	5.01	116.75	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	TYR	Sidechain

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	3322	0	3321	86	0
2	A	44	0	24	2	0
3	A	19	0	12	1	0
4	A	8	0	16	0	0
5	A	213	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3606	0	3373	86	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 13.

All (86) 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:143:TYR:HB3	1:A:146:LEU:HD13	1.51	0.92
1:A:128:ILE:HD11	1:A:139:ILE:HD12	1.54	0.86
1:A:215:VAL:H	1:A:270:ASN:HD22	1.21	0.85
1:A:188:LYS:HE2	5:A:1100:HOH:O	1.77	0.85
1:A:410:THR:H	1:A:413:GLN:HE21	1.28	0.81
1:A:426:LYS:HG2	1:A:430:TYR:CD2	2.17	0.80
1:A:143:TYR:O	1:A:146:LEU:HD13	1.84	0.77
1:A:146:LEU:HD12	1:A:146:LEU:N	2.02	0.73
1:A:125:LEU:H	1:A:125:LEU:HD13	1.55	0.72
1:A:191:ASN:HD22	1:A:191:ASN:H	1.36	0.72
1:A:191:ASN:HD22	1:A:191:ASN:N	1.89	0.71
1:A:23:ASP:HB3	5:A:1111:HOH:O	1.90	0.70
1:A:125:LEU:O	1:A:125:LEU:HD22	1.91	0.70
1:A:143:TYR:HB3	1:A:146:LEU:CD1	2.20	0.70
1:A:188:LYS:CE	5:A:1100:HOH:O	2.35	0.69
1:A:106:THR:OG1	1:A:109:GLU:HG3	1.93	0.68
1:A:374:THR:HG22	1:A:375:HIS:CE1	2.30	0.66
1:A:118:LEU:HA	1:A:125:LEU:HD12	1.78	0.65
1:A:33:MET:HE1	1:A:36:ARG:CZ	2.30	0.62
1:A:184:VAL:HG21	1:A:432:TYR:CE1	2.37	0.60
1:A:370:ILE:O	1:A:374:THR:HB	2.03	0.59
1:A:346:ASN:H	1:A:346:ASN:HD22	1.51	0.58
1:A:75:GLN:HG3	1:A:120:PHE:CE2	2.39	0.57
1:A:411:GLU:O	1:A:415:GLN:HG3	2.05	0.57
1:A:346:ASN:HD21	2:A:433:NAD:H72N	1.51	0.57
1:A:39:TYR:CD2	1:A:44:PRO:HG3	2.41	0.56
1:A:108:GLU:H	1:A:108:GLU:CD	2.11	0.56
1:A:346:ASN:HD22	1:A:346:ASN:N	2.03	0.56
1:A:146:LEU:N	1:A:146:LEU:CD1	2.69	0.55
1:A:426:LYS:HG2	1:A:430:TYR:CG	2.41	0.55
1:A:186:LYS:HZ2	1:A:191:ASN:HD21	1.55	0.53
1:A:380:PRO:O	1:A:384:HIS:HE1	1.90	0.53
1:A:387:PRO:HD2	1:A:390:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLU:CD	1:A:108:GLU:N	2.68	0.52
1:A:73:GLU:HG3	5:A:1061:HOH:O	2.10	0.52
1:A:19:ARG:NH1	1:A:22:LEU:HD12	2.24	0.51
1:A:396:GLU:HA	1:A:399:LEU:HD22	1.93	0.51
1:A:54:LEU:O	1:A:55:HIS:C	2.53	0.51
1:A:143:TYR:CB	1:A:146:LEU:HD13	2.33	0.50
1:A:161:VAL:HG21	1:A:179:ASN:OD1	2.12	0.50
1:A:125:LEU:HD23	1:A:150:ILE:HG12	1.94	0.49
1:A:125:LEU:HD21	1:A:150:ILE:HD11	1.93	0.49
1:A:181:ASN:HA	1:A:186:LYS:HD2	1.93	0.49
1:A:178:ILE:HD12	1:A:372:LEU:HD22	1.94	0.48
1:A:168:MET:SD	1:A:382:GLY:HA2	2.53	0.48
1:A:175:VAL:HG13	1:A:176:PRO:HD2	1.95	0.48
1:A:226:LYS:HZ3	1:A:251:GLN:HE22	1.62	0.48
1:A:274:THR:HB	1:A:305:GLU:OE1	2.13	0.48
1:A:415:GLN:NE2	5:A:1112:HOH:O	2.46	0.48
1:A:410:THR:H	1:A:413:GLN:NE2	2.03	0.48
1:A:191:ASN:N	1:A:191:ASN:ND2	2.60	0.47
1:A:309:LYS:O	1:A:313:GLU:HG3	2.14	0.47
1:A:317:GLU:HB2	1:A:329:ARG:HB3	1.96	0.46
1:A:388:LYS:O	1:A:392:GLU:HG3	2.16	0.46
1:A:125:LEU:H	1:A:125:LEU:CD1	2.26	0.46
1:A:58:VAL:H	1:A:85:GLN:NE2	2.14	0.46
1:A:206:ALA:O	1:A:322:LYS:HE3	2.15	0.46
1:A:233:ARG:HG3	5:A:1048:HOH:O	2.14	0.46
1:A:368:ALA:O	1:A:372:LEU:HD22	2.16	0.46
1:A:137:ASN:O	1:A:141:THR:HG23	2.16	0.45
1:A:380:PRO:O	1:A:384:HIS:CE1	2.69	0.45
1:A:186:LYS:HD3	1:A:186:LYS:C	2.41	0.45
1:A:359:SER:CB	1:A:398:HIS:HE2	2.30	0.45
1:A:7:TYR:C	1:A:7:TYR:CD1	2.94	0.45
1:A:155:GLU:O	1:A:180:VAL:HB	2.16	0.45
1:A:92:ILE:HG23	1:A:97:ILE:HB	1.99	0.45
1:A:374:THR:CG2	1:A:375:HIS:CE1	3.00	0.44
1:A:55:HIS:CD2	3:A:434:NOC:H5'2	2.53	0.44
1:A:186:LYS:NZ	1:A:191:ASN:HD21	2.15	0.44
1:A:248:ASN:HA	1:A:251:GLN:HE21	1.82	0.44
1:A:191:ASN:H	1:A:191:ASN:ND2	2.11	0.43
1:A:134:ASP:HB2	5:A:1018:HOH:O	2.18	0.43
1:A:226:LYS:NZ	1:A:251:GLN:HE22	2.16	0.43
1:A:45:LEU:HB3	1:A:72:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASN:CG	2:A:433:NAD:H5N	2.43	0.43
1:A:198:SER:OG	1:A:353:HIS:HD2	2.01	0.43
1:A:94:LYS:C	1:A:96:GLY:H	2.26	0.42
1:A:162:HIS:CE1	5:A:998:HOH:O	2.72	0.42
1:A:173:LEU:HD22	1:A:175:VAL:H	1.84	0.42
1:A:188:LYS:HD3	5:A:1100:HOH:O	2.20	0.42
1:A:248:ASN:HD22	1:A:248:ASN:H	1.68	0.42
1:A:279:ILE:HG22	1:A:304:VAL:HB	2.02	0.41
1:A:143:TYR:N	1:A:144:PRO:CD	2.82	0.41
1:A:185:THR:HA	1:A:189:PHE:CD1	2.56	0.41
1:A:211:ILE:HG22	1:A:237:ALA:HB2	2.04	0.40
1:A:147:LEU:HB2	1:A:148:PRO:HD3	2.04	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	428/432 (99%)	414 (97%)	13 (3%)	1 (0%)	43	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	HIS

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	352/356 (99%)	331 (94%)	21 (6%)	17	14

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	94	LYS
1	A	108	GLU
1	A	111	LEU
1	A	125	LEU
1	A	146	LEU
1	A	161	VAL
1	A	173	LEU
1	A	190	ASP
1	A	191	ASN
1	A	210	MET
1	A	254	MET
1	A	283	LEU
1	A	346	ASN
1	A	372	LEU
1	A	374	THR
1	A	399	LEU
1	A	403	ASN
1	A	409	LEU
1	A	411	GLU
1	A	412	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	85	GLN
1	A	162	HIS
1	A	181	ASN
1	A	191	ASN
1	A	248	ASN
1	A	251	GLN
1	A	267	GLN
1	A	270	ASN
1	A	324	GLN

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Mol	Chain	Res	Type
1	A	346	ASN
1	A	353	HIS
1	A	365	GLN
1	A	369	GLN
1	A	384	HIS
1	A	413	GLN
1	A	415	GLN

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 ⓘ

4 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	$\# Z > 2$
4	IPA	A	900	-	3,3,3	1.00	0	3,3,3	0.49	0
4	IPA	A	901	-	3,3,3	0.86	0	3,3,3	0.30	0
2	NAD	A	433	-	46,48,48	5.52	31 (67%)	64,73,73	3.18	26 (40%)
3	NOC	A	434	-	21,21,21	3.04	7 (33%)	30,31,31	2.05	10 (33%)

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	A	433	-	-	6/30/62/62	0/5/5/5
3	NOC	A	434	-	1/1/4/4	4/6/22/22	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	433	NAD	C4N-C3N	15.67	1.63	1.39
2	A	433	NAD	PA-O3	12.51	1.73	1.59
2	A	433	NAD	C8A-N9A	12.05	1.58	1.37
2	A	433	NAD	C2N-N1N	9.46	1.45	1.35
3	A	434	NOC	O3'-C3'	-8.75	1.21	1.43
2	A	433	NAD	C5A-C4A	8.07	1.53	1.39
2	A	433	NAD	C2A-N1A	7.95	1.48	1.33
2	A	433	NAD	O4B-C4B	-7.92	1.27	1.45
2	A	433	NAD	O4D-C1D	7.65	1.50	1.40
2	A	433	NAD	PN-O5D	-7.46	1.30	1.59
2	A	433	NAD	C4A-N9A	-7.02	1.23	1.37
2	A	433	NAD	O5B-C5B	-6.25	1.20	1.44
3	A	434	NOC	C5'-C4'	-5.89	1.38	1.53
2	A	433	NAD	C6A-N1A	5.79	1.51	1.35
2	A	433	NAD	C5A-N7A	-5.53	1.29	1.39
2	A	433	NAD	C6N-N1N	5.37	1.47	1.35
2	A	433	NAD	C3B-C4B	-5.16	1.39	1.53
2	A	433	NAD	C6N-C5N	5.02	1.49	1.38
3	A	434	NOC	C6'-C4'	-5.01	1.42	1.52
2	A	433	NAD	C3N-C7N	4.70	1.57	1.50
2	A	433	NAD	C2B-C1B	-4.67	1.38	1.53
2	A	433	NAD	C3D-C4D	4.59	1.64	1.53
2	A	433	NAD	PN-O3	4.58	1.64	1.59
2	A	433	NAD	O3B-C3B	4.51	1.54	1.43
2	A	433	NAD	C2N-C3N	4.05	1.45	1.39
3	A	434	NOC	C2'-C1'	3.96	1.58	1.53
2	A	433	NAD	O4D-C4D	3.80	1.53	1.45
2	A	433	NAD	C5A-C6A	3.51	1.50	1.41
2	A	433	NAD	O4B-C1B	3.36	1.49	1.42
2	A	433	NAD	O2B-C2B	-3.05	1.35	1.43
2	A	433	NAD	PA-O2A	-2.84	1.42	1.55
2	A	433	NAD	C1B-N9A	-2.74	1.38	1.46
3	A	434	NOC	C5-C4	2.64	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	434	NOC	C4-N3	2.46	1.39	1.34
2	A	433	NAD	C6A-N6A	-2.34	1.28	1.34
3	A	434	NOC	C4'-C3'	-2.29	1.47	1.54
2	A	433	NAD	C5B-C4B	-2.28	1.44	1.51
2	A	433	NAD	C4A-N3A	2.13	1.38	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	433	NAD	C6N-N1N-C2N	10.25	130.60	121.88
2	A	433	NAD	O7N-C7N-C3N	-8.62	109.05	119.60
2	A	433	NAD	PA-O5B-C5B	8.24	168.59	121.35
2	A	433	NAD	O5B-C5B-C4B	6.37	130.67	108.99
3	A	434	NOC	O3'-C3'-C4'	6.21	128.77	112.56
2	A	433	NAD	C2N-C3N-C4N	5.16	124.26	118.26
2	A	433	NAD	O5D-C5D-C4D	5.08	126.29	108.99
2	A	433	NAD	C5N-C4N-C3N	-4.56	115.89	120.36
2	A	433	NAD	N3A-C2A-N1A	-4.44	121.86	128.58
2	A	433	NAD	C2N-C3N-C7N	-4.43	106.66	119.46
2	A	433	NAD	O2A-PA-O5B	4.38	127.44	107.57
2	A	433	NAD	C3N-C7N-N7N	4.26	122.99	117.74
2	A	433	NAD	O2A-PA-O3	4.16	118.50	107.27
2	A	433	NAD	O2N-PN-O3	4.06	118.26	107.27
2	A	433	NAD	C2B-C3B-C4B	3.96	110.27	102.61
2	A	433	NAD	C2A-N3A-C4A	3.65	120.74	111.83
2	A	433	NAD	C5N-C6N-N1N	-3.63	115.43	120.38
3	A	434	NOC	C5'-C4'-C3'	3.61	112.04	102.89
2	A	433	NAD	O3-PA-O1A	-3.56	100.00	110.70
3	A	434	NOC	C5'-C4'-C6'	3.38	123.69	112.88
2	A	433	NAD	O7N-C7N-N7N	3.33	127.43	122.62
2	A	433	NAD	C2N-N1N-C1D	-3.26	111.93	119.13
2	A	433	NAD	C4A-C5A-N7A	3.24	114.29	110.58
3	A	434	NOC	O3'-C3'-C2'	3.13	121.84	111.82
3	A	434	NOC	C5'-C1'-N9	2.95	117.13	113.40
2	A	433	NAD	C4N-C3N-C7N	2.77	128.59	121.06
2	A	433	NAD	O2B-C2B-C1B	2.67	119.30	110.10
2	A	433	NAD	O5B-PA-O1A	-2.53	98.92	108.94
3	A	434	NOC	C5'-C1'-C2'	-2.48	99.97	104.22
2	A	433	NAD	C5D-C4D-C3D	-2.32	106.85	115.21
3	A	434	NOC	C4'-C5'-C1'	2.27	109.79	102.41
2	A	433	NAD	N9A-C8A-N7A	-2.14	110.89	113.94
3	A	434	NOC	C6'-C4'-C3'	2.10	124.02	113.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	434	NOC	C2-N1-C6	2.08	122.15	118.73
3	A	434	NOC	C4-C5-N7	-2.02	108.28	110.58
2	A	433	NAD	C2A-N1A-C6A	2.01	122.04	118.73

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	434	NOC	C4'

All (10) torsion outliers are listed below:

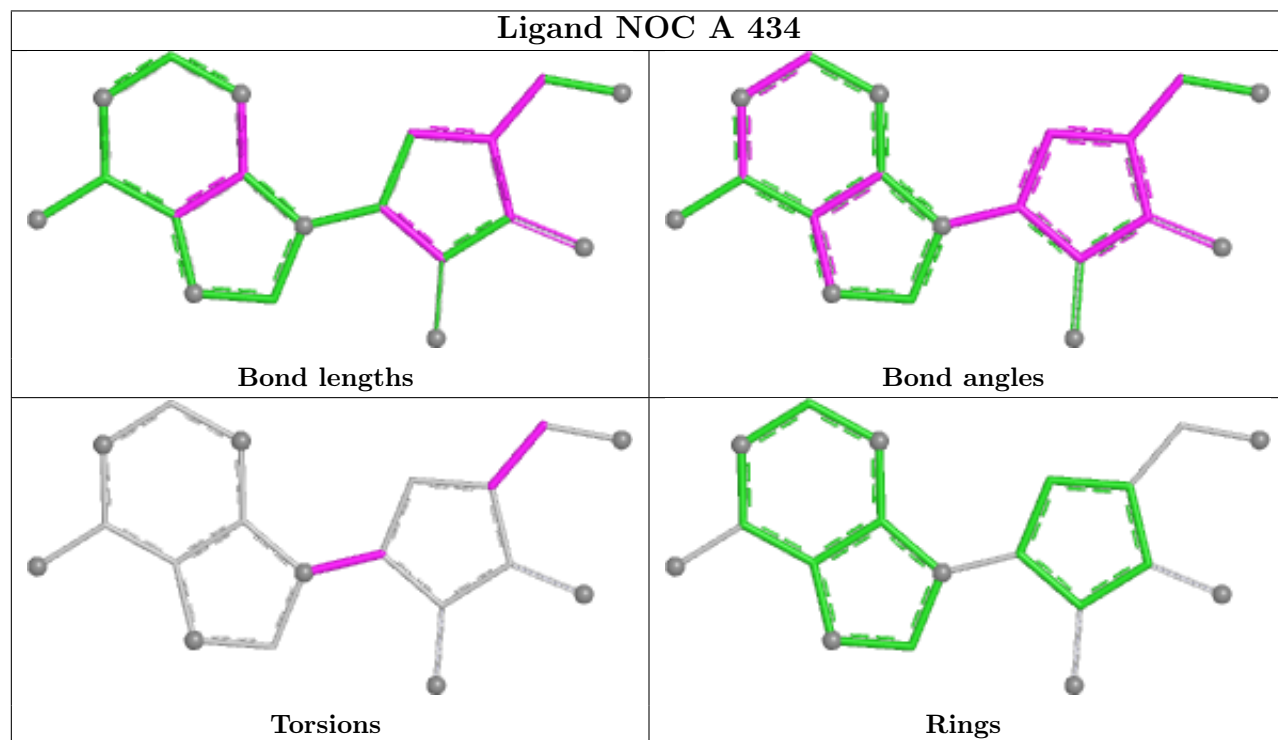
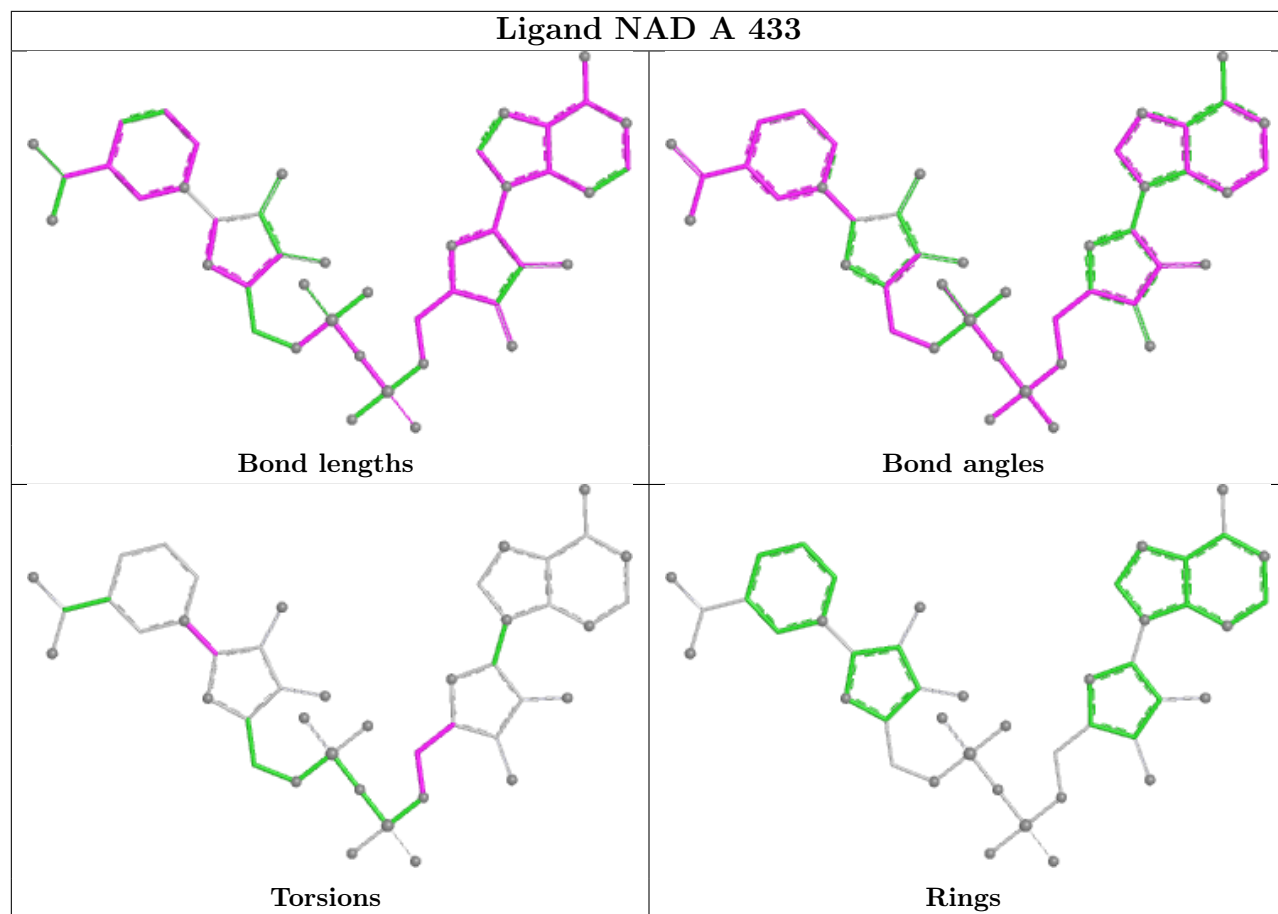
Mol	Chain	Res	Type	Atoms
2	A	433	NAD	O4D-C1D-N1N-C2N
2	A	433	NAD	O4D-C1D-N1N-C6N
2	A	433	NAD	C2D-C1D-N1N-C2N
2	A	433	NAD	C2D-C1D-N1N-C6N
3	A	434	NOC	C3'-C4'-C6'-O6'
3	A	434	NOC	C2'-C1'-N9-C4
3	A	434	NOC	C5'-C1'-N9-C4
2	A	433	NAD	C4B-C5B-O5B-PA
3	A	434	NOC	C5'-C1'-N9-C8
2	A	433	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	433	NAD	2	0
3	A	434	NOC	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

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	430/432 (99%)	0.32	19 (4%) 39 38	14, 27, 44, 51	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	TYR	4.7
1	A	162	HIS	4.4
1	A	144	PRO	3.3
1	A	172	ILE	3.1
1	A	123	GLY	3.0
1	A	372	LEU	2.9
1	A	171	GLY	2.9
1	A	41	ALA	2.7
1	A	382	GLY	2.7
1	A	374	THR	2.5
1	A	166	LYS	2.5
1	A	139	ILE	2.5
1	A	377	ASP	2.4
1	A	125	LEU	2.3
1	A	147	LEU	2.3
1	A	120	PHE	2.3
1	A	415	GLN	2.2
1	A	45	LEU	2.2
1	A	17	TRP	2.1

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 [i](#)

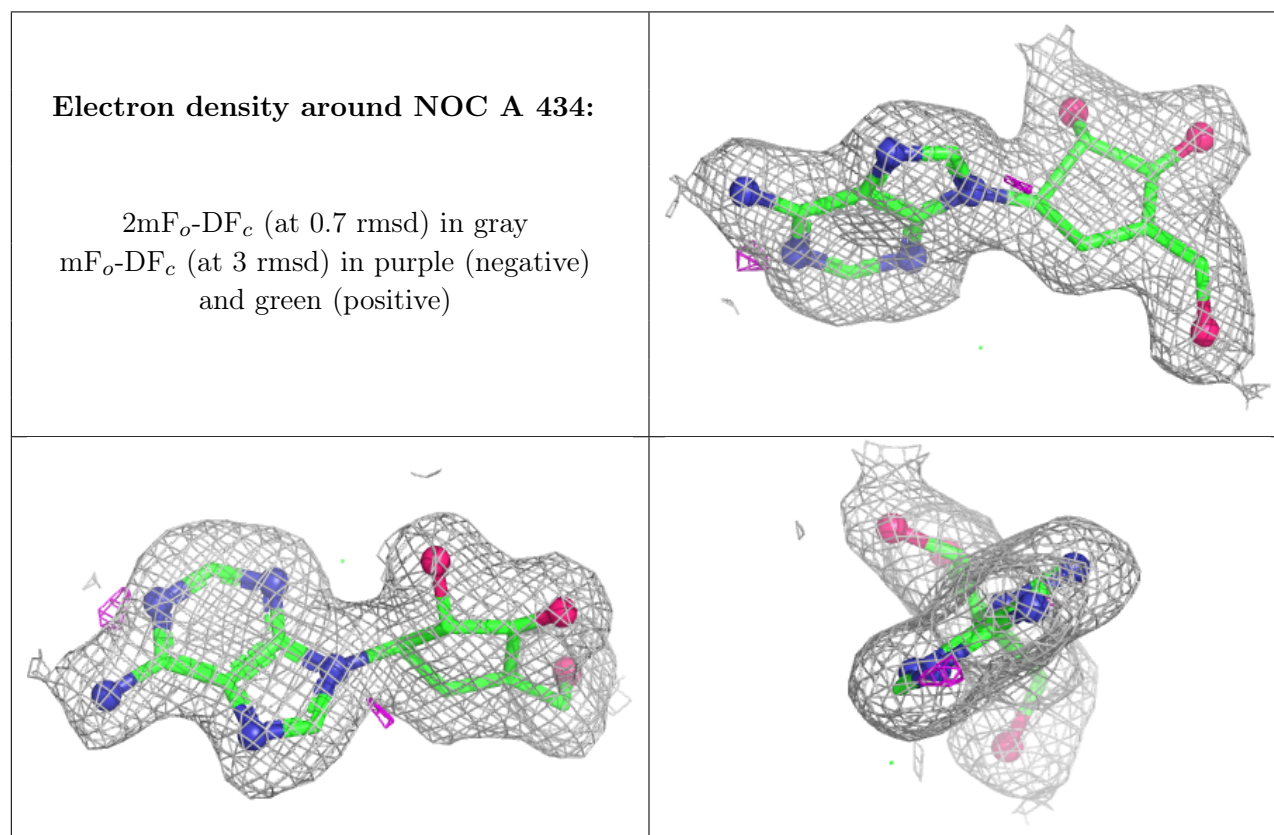
There are no oligosaccharides in this entry.

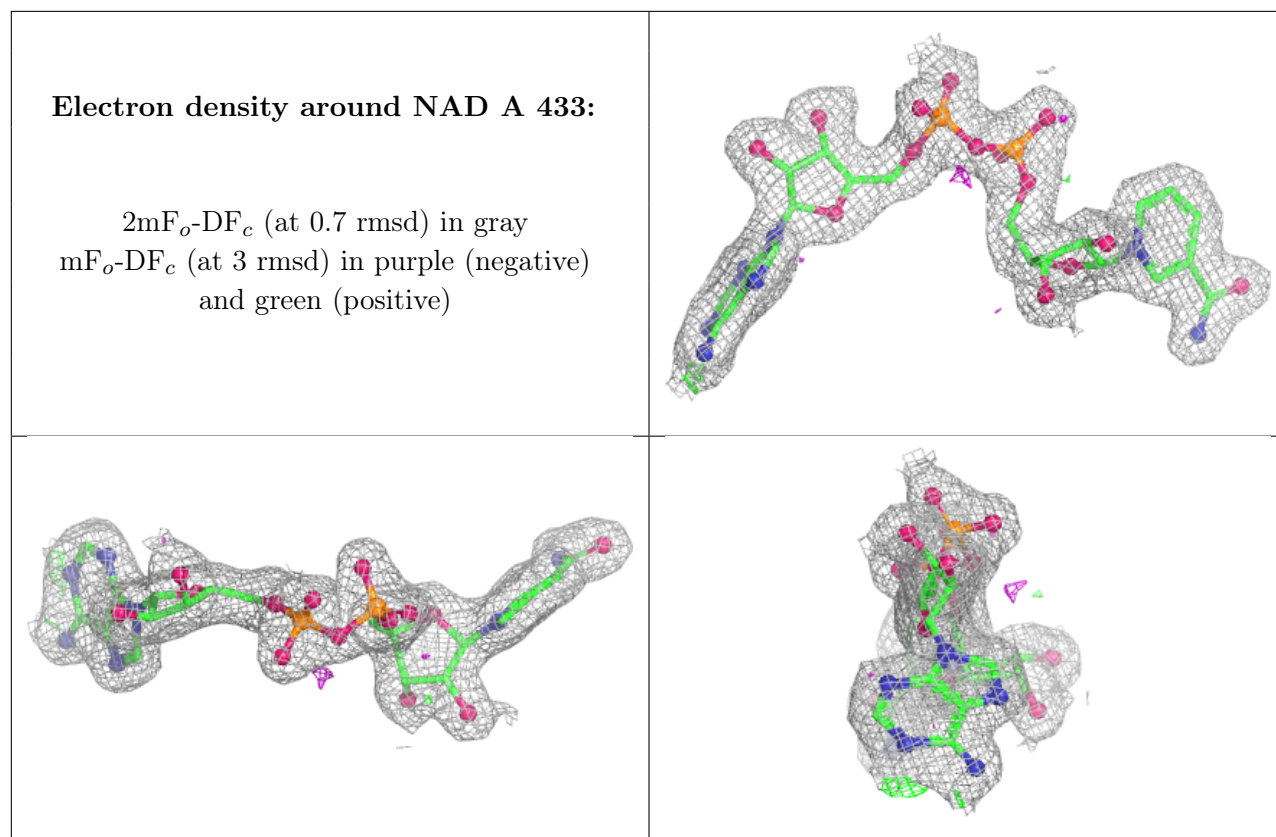
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
4	IPA	A	901	4/4	0.74	0.16	33,34,34,34	0
4	IPA	A	900	4/4	0.84	0.18	27,27,28,28	0
3	NOC	A	434	19/19	0.94	0.07	18,19,19,19	0
2	NAD	A	433	44/44	0.97	0.06	16,19,20,21	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.