



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:49 AM UTC

PDB ID : 9JHZ / pdb_00009jhz
Title : 3-Hydroxybutyryl-CoA dehydrogenase mutant(S117A) with acetoacetyl CoA and NAD
Authors : Yang, J.W.; Jeon, H.J.; Park, S.H.; Kim, S.H.; Hwang, K.Y.
Deposited on : 2024-09-10
Resolution : 2.20 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

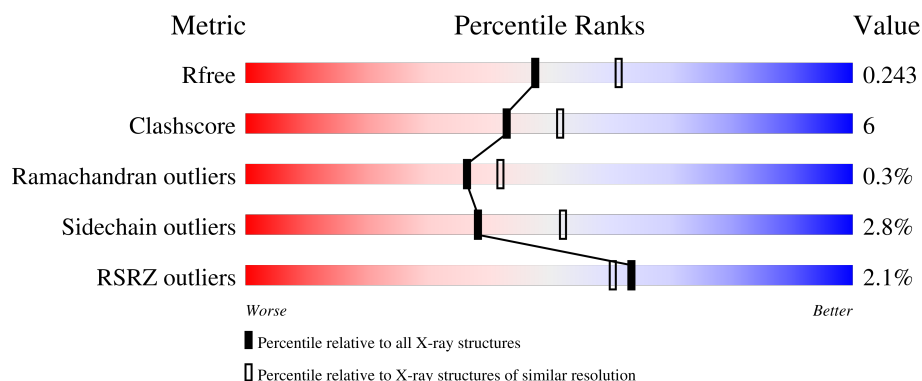
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	291	 89% 9% .
1	B	291	 6% 79% 18% ...
1	C	291	 88% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6821 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.

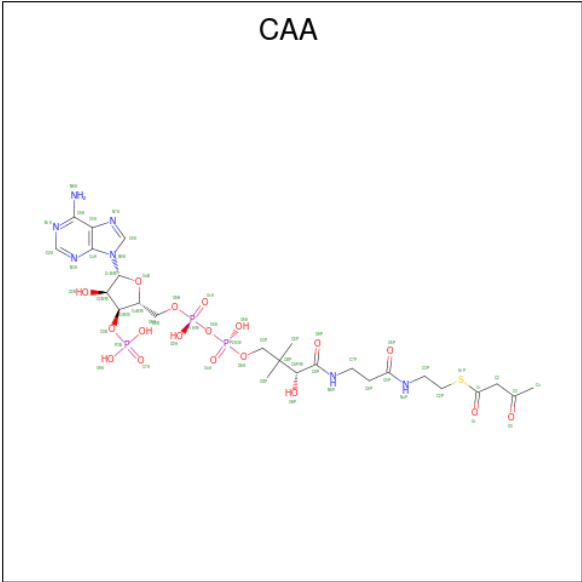
- Molecule 1 is a protein called 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	290	Total	C	N	O	S	0	0	0
			2167	1376	365	406	20			
1	A	288	Total	C	N	O	S	0	0	0
			2153	1368	362	403	20			
1	B	289	Total	C	N	O	S	0	0	0
			2162	1373	364	405	20			

There are 6 discrepancies between the modelled and reference sequences:

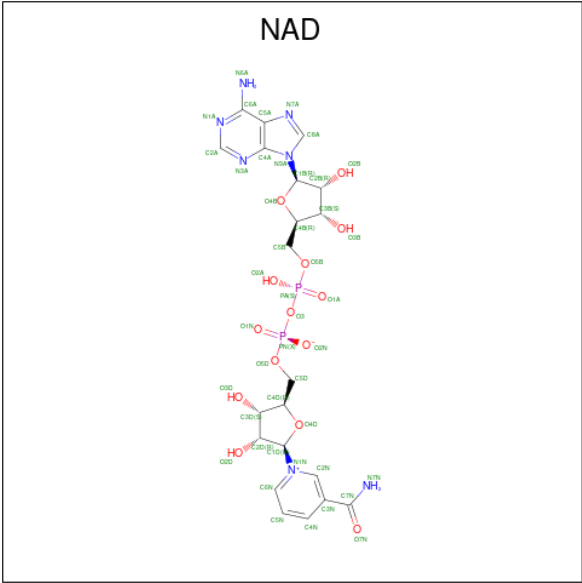
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	expression tag	UNP C7H5K9
C	117	ALA	SER	engineered mutation	UNP C7H5K9
A	0	ALA	-	expression tag	UNP C7H5K9
A	117	ALA	SER	engineered mutation	UNP C7H5K9
B	0	ALA	-	expression tag	UNP C7H5K9
B	117	ALA	SER	engineered mutation	UNP C7H5K9

- Molecule 2 is ACETOACETYL-COENZYME A (CCD ID: CAA) (formula: $C_{25}H_{40}N_7O_{18}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	54	25	7	18	3	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



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

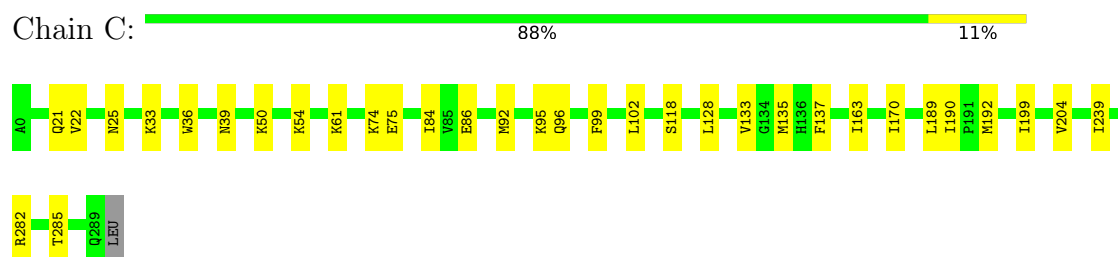
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	83	Total 83	O 83	0	0
4	A	102	Total 102	O 102	0	0
4	B	56	Total 56	O 56	0	0

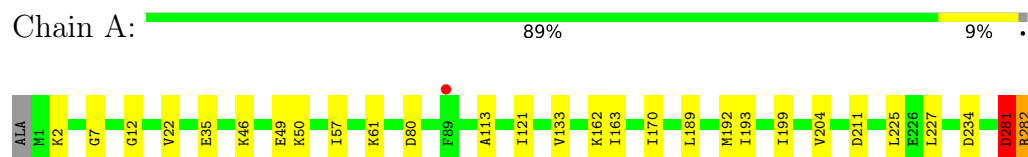
3 Residue-property plots [i](#)

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.

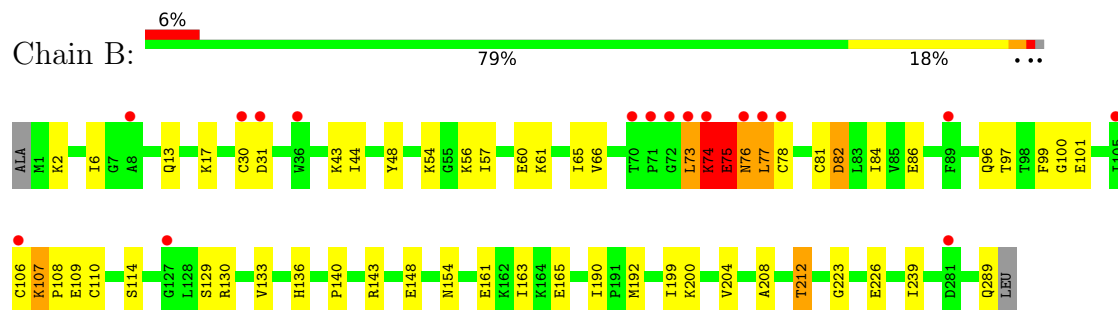
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein



- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein



- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase, NAD binding domain protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	90.56Å 90.56Å 212.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.28 – 2.20 45.28 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.28-2.20) 99.0 (45.28-2.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.197 , 0.243 0.198 , 0.243	Depositor DCC
R_{free} test set	1994 reflections (3.91%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6821	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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, CAA

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	0.16	0/2184	0.35	1/2942 (0.0%)
1	B	0.33	0/2193	0.52	0/2954
1	C	0.21	0/2198	0.38	0/2961
All	All	0.25	0/6575	0.43	1/8857 (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	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ARG	N-CA-C	-5.88	107.34	114.75

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	ARG	Sidechain
1	C	282	ARG	Sidechain

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	2153	0	2227	19	0
1	B	2162	0	2235	42	0
1	C	2167	0	2240	20	0
2	B	54	0	35	4	0
3	B	44	0	25	2	0
4	A	102	0	0	1	0
4	B	56	0	0	3	0
4	C	83	0	0	3	0
All	All	6821	0	6762	82	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 (82) 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)
3:B:402:NAD:O4B	3:B:402:NAD:C1B	1.65	1.18
1:B:73:LEU:HD22	1:B:76:ASN:HB2	1.65	0.79
1:B:13:GLN:HB3	1:B:44:ILE:HD11	1.63	0.78
1:B:54:LYS:NZ	2:B:401:CAA:O9A	2.23	0.71
1:B:289:GLN:HG3	4:B:541:HOH:O	1.95	0.66
1:B:30:CYS:HB3	1:B:74:LYS:HA	1.78	0.66
1:B:100:GLY:O	4:B:501:HOH:O	2.15	0.65
1:B:199:ILE:HG23	1:B:204:VAL:HB	1.78	0.65
1:C:39:ASN:ND2	4:C:301:HOH:O	2.29	0.64
1:B:208:ALA:O	1:B:212:THR:HG23	2.01	0.61
1:B:57:ILE:HD11	2:B:401:CAA:N6A	2.16	0.60
1:B:133:VAL:HG11	1:B:163:ILE:HG13	1.84	0.60
1:B:75:GLU:C	1:B:77:LEU:H	2.09	0.59
1:B:17:LYS:HD2	1:B:44:ILE:HD12	1.83	0.59
1:B:97:THR:O	1:B:101:GLU:HG3	2.03	0.58
1:B:73:LEU:O	1:B:74:LYS:HB3	2.04	0.58
1:C:189:LEU:O	1:C:192:MET:HB2	2.04	0.56
1:B:48:TYR:CE2	1:B:65:ILE:HD11	2.41	0.56
1:C:74:LYS:NZ	1:C:75:GLU:OE2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:LYS:HA	1:C:50:LYS:HE2	1.87	0.55
1:B:57:ILE:HD11	2:B:401:CAA:H62A	1.72	0.55
1:B:223:GLY:N	1:B:226:GLU:OE2	2.29	0.55
1:B:161:GLU:O	1:B:165:GLU:HG3	2.07	0.54
1:B:140:PRO:HG2	1:B:143:ARG:HB2	1.90	0.54
1:B:86:GLU:HG2	1:B:99:PHE:CE2	2.44	0.53
1:C:50:LYS:O	1:C:54:LYS:HG3	2.08	0.53
1:B:31:ASP:OD2	3:B:402:NAD:H1B	2.09	0.52
1:B:200:LYS:NZ	4:B:504:HOH:O	2.41	0.52
1:B:75:GLU:C	1:B:77:LEU:N	2.69	0.51
1:B:86:GLU:HG3	1:B:114:SER:HA	1.91	0.51
1:B:136:HIS:HB3	1:B:148:GLU:HB2	1.92	0.51
1:C:33:LYS:HE2	1:C:36:TRP:CZ2	2.45	0.51
1:C:22:VAL:HB	1:C:25:ASN:HD22	1.76	0.51
1:C:22:VAL:HB	1:C:25:ASN:ND2	2.27	0.50
1:B:78:CYS:HA	1:B:81:CYS:SG	2.51	0.50
1:C:199:ILE:HG23	1:C:204:VAL:HB	1.92	0.50
1:B:75:GLU:O	1:B:77:LEU:N	2.39	0.50
1:C:84:ILE:HG21	1:C:102:LEU:HD13	1.95	0.49
1:B:56:LYS:HG3	2:B:401:CAA:H2B	1.95	0.49
1:C:135:MET:HE2	1:C:137:PHE:CZ	2.47	0.48
1:C:190:ILE:HG13	1:C:239:ILE:HG21	1.95	0.48
1:B:107:LYS:HB3	1:B:107:LYS:HE3	1.65	0.48
1:C:86:GLU:OE1	1:C:95:LYS:HD3	2.13	0.47
1:A:50:LYS:HB3	1:A:50:LYS:HE2	1.55	0.47
1:A:189:LEU:O	1:A:192:MET:HB3	2.14	0.47
1:B:6:ILE:HB	1:B:86:GLU:HA	1.96	0.47
1:A:199:ILE:HG23	1:A:204:VAL:HB	1.96	0.46
1:A:133:VAL:HG11	1:A:163:ILE:HG13	1.96	0.46
1:A:22:VAL:HG21	1:A:170:ILE:HA	1.99	0.45
1:B:2:LYS:HG3	1:B:81:CYS:HA	1.99	0.45
1:C:61:LYS:NZ	4:C:308:HOH:O	2.46	0.45
1:B:73:LEU:CD2	1:B:76:ASN:HB2	2.42	0.45
1:A:234:ASP:OD1	1:A:234:ASP:N	2.49	0.45
1:B:73:LEU:HD23	1:B:75:GLU:H	1.81	0.45
1:B:96:GLN:O	1:B:100:GLY:N	2.46	0.45
1:B:82:ASP:N	1:B:82:ASP:OD1	2.51	0.44
1:A:35:GLU:CD	1:A:35:GLU:H	2.26	0.44
1:C:99:PHE:HB3	1:C:128:LEU:HD11	2.00	0.44
1:A:121:ILE:HD13	1:A:121:ILE:HA	1.84	0.43
1:A:162:LYS:NZ	4:A:313:HOH:O	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:PRO:O	1:B:130:ARG:NH1	2.51	0.43
1:C:22:VAL:HG21	1:C:170:ILE:HA	2.00	0.43
1:A:57:ILE:HD11	1:A:61:LYS:HG2	2.01	0.43
1:A:46:LYS:HA	1:A:49:GLU:HG3	2.01	0.43
1:A:281:ASP:OD1	1:A:281:ASP:N	2.43	0.43
1:C:192:MET:HB3	1:C:192:MET:HE3	1.64	0.42
1:B:96:GLN:HE21	1:B:96:GLN:HB3	1.58	0.42
1:B:61:LYS:HA	1:B:61:LYS:HD2	1.72	0.42
1:B:190:ILE:HG13	1:B:239:ILE:HG21	2.01	0.42
1:B:84:ILE:HD13	1:B:84:ILE:HA	1.77	0.42
1:A:192:MET:HE2	1:A:192:MET:HB2	1.90	0.42
1:A:189:LEU:HA	1:A:192:MET:HE3	2.01	0.42
1:A:2:LYS:NZ	1:A:80:ASP:OD2	2.53	0.42
1:A:211:ASP:OD2	1:A:225:LEU:HB2	2.19	0.42
1:C:133:VAL:HG11	1:C:163:ILE:HG13	2.01	0.41
1:A:7:GLY:O	1:A:12:GLY:HA3	2.20	0.41
1:B:2:LYS:HA	1:B:2:LYS:HD3	1.96	0.41
1:B:192:MET:HE2	1:B:192:MET:HB3	1.90	0.41
1:C:21:GLN:NE2	4:C:303:HOH:O	2.37	0.41
1:A:113:ALA:HA	1:A:133:VAL:O	2.21	0.41
1:A:193:ILE:HD11	1:A:227:LEU:HD23	2.04	0.40
1:C:92:MET:O	1:C:96:GLN:HG3	2.21	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	286/291 (98%)	280 (98%)	5 (2%)	1 (0%)	36	42
1	B	287/291 (99%)	272 (95%)	13 (4%)	2 (1%)	18	19
1	C	288/291 (99%)	282 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	861/873 (99%)	834 (97%)	24 (3%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ASP
1	B	74	LYS
1	B	75	GLU

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	228/230 (99%)	227 (100%)	1 (0%)	84	92
1	B	229/230 (100%)	213 (93%)	16 (7%)	14	16
1	C	229/230 (100%)	227 (99%)	2 (1%)	70	84
All	All	686/690 (99%)	667 (97%)	19 (3%)	38	52

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	118	SER
1	C	285	THR
1	A	281	ASP
1	B	43	LYS
1	B	60	GLU
1	B	66	VAL
1	B	73	LEU
1	B	74	LYS
1	B	75	GLU
1	B	76	ASN
1	B	77	LEU
1	B	82	ASP
1	B	106	CYS

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Mol	Chain	Res	Type
1	B	107	LYS
1	B	109	GLU
1	B	110	CYS
1	B	129	SER
1	B	154	ASN
1	B	212	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	154	ASN
1	C	245	HIS
1	A	178	ASN
1	A	279	ASN
1	B	96	GLN
1	B	176	GLN

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](#)

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
2	CAA	B	401	-	53,56,56	2.94	16 (30%)	77,83,83	2.24	18 (23%)
3	NAD	B	402	-	46,48,48	5.51	26 (56%)	64,73,73	2.47	18 (28%)

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	CAA	B	401	-	-	14/55/71/71	0/3/3/3
3	NAD	B	402	-	-	12/30/62/62	0/5/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NAD	O4D-C1D	16.56	1.62	1.40
3	B	402	NAD	C2N-N1N	15.13	1.51	1.35
3	B	402	NAD	O4B-C1B	10.18	1.65	1.42
3	B	402	NAD	C2N-C3N	9.45	1.54	1.39
3	B	402	NAD	C7N-N7N	8.98	1.49	1.33
2	B	401	CAA	C3B-C4B	-8.94	1.29	1.52
3	B	402	NAD	O4D-C4D	-8.28	1.26	1.45
2	B	401	CAA	C2B-C1B	-8.23	1.27	1.53
3	B	402	NAD	C4N-C3N	8.14	1.51	1.39
2	B	401	CAA	O4B-C1B	8.11	1.60	1.42
3	B	402	NAD	C5N-C4N	8.05	1.52	1.38
2	B	401	CAA	C2B-C3B	7.89	1.70	1.53
3	B	402	NAD	PN-O3	7.88	1.68	1.59
3	B	402	NAD	C6N-C5N	7.79	1.54	1.38
3	B	402	NAD	C6N-N1N	7.03	1.51	1.35
3	B	402	NAD	C2B-C1B	-6.89	1.31	1.53
3	B	402	NAD	O4B-C4B	-6.06	1.31	1.45
3	B	402	NAD	PA-O3	5.58	1.65	1.59
2	B	401	CAA	C9P-N8P	5.14	1.45	1.33
3	B	402	NAD	C6A-N6A	4.97	1.46	1.34
2	B	401	CAA	P2A-O3A	4.81	1.64	1.59
2	B	401	CAA	C5P-N4P	4.69	1.44	1.33
2	B	401	CAA	C6A-N6A	4.34	1.45	1.34
2	B	401	CAA	P1A-O3A	4.25	1.64	1.59
3	B	402	NAD	O3B-C3B	-3.46	1.34	1.43
2	B	401	CAA	O4B-C4B	3.22	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NAD	O2D-C2D	3.19	1.50	1.43
3	B	402	NAD	O2B-C2B	3.15	1.50	1.43
2	B	401	CAA	P3B-O3B	3.13	1.65	1.59
3	B	402	NAD	C3N-C7N	2.88	1.54	1.50
2	B	401	CAA	C8A-N9A	-2.81	1.32	1.37
3	B	402	NAD	O7N-C7N	-2.80	1.18	1.24
3	B	402	NAD	C5D-C4D	2.68	1.59	1.51
2	B	401	CAA	O9P-C9P	-2.48	1.18	1.23
3	B	402	NAD	PN-O5D	2.47	1.69	1.59
3	B	402	NAD	C8A-N9A	-2.46	1.33	1.37
3	B	402	NAD	C5A-N7A	-2.44	1.34	1.39
2	B	401	CAA	C5A-N7A	-2.36	1.34	1.39
3	B	402	NAD	PA-O5B	2.27	1.68	1.59
3	B	402	NAD	C3D-C4D	2.17	1.58	1.53
2	B	401	CAA	O5P-C5P	-2.11	1.19	1.23
2	B	401	CAA	C1-S1P	2.00	1.81	1.76

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAD	C6N-N1N-C2N	-10.94	112.57	121.88
2	B	401	CAA	C4B-O4B-C1B	-10.69	85.86	109.47
3	B	402	NAD	C6N-N1N-C1D	-5.65	108.64	119.73
3	B	402	NAD	C5A-C4A-N3A	-5.62	118.97	126.72
2	B	401	CAA	C5A-C4A-N3A	-5.23	119.51	126.72
3	B	402	NAD	C2N-C3N-C4N	-4.79	112.69	118.26
3	B	402	NAD	C4N-C3N-C7N	-4.78	108.05	121.06
2	B	401	CAA	C2B-C3B-C4B	-4.59	95.21	103.24
2	B	401	CAA	N3A-C2A-N1A	-4.50	121.77	128.58
2	B	401	CAA	C2-C1-S1P	4.31	119.10	113.63
3	B	402	NAD	N3A-C4A-N9A	4.09	134.13	127.17
2	B	401	CAA	C2B-C1B-N9A	3.81	122.78	113.30
2	B	401	CAA	N3A-C4A-N9A	3.76	133.56	127.17
3	B	402	NAD	N3A-C2A-N1A	-3.69	122.99	128.58
2	B	401	CAA	C2A-N3A-C4A	3.60	120.63	111.83
3	B	402	NAD	C2A-N3A-C4A	3.55	120.51	111.83
3	B	402	NAD	C4A-C5A-N7A	-3.33	106.78	110.58
3	B	402	NAD	C2N-N1N-C1D	-3.32	111.81	119.13
2	B	401	CAA	C7P-C6P-C5P	-3.28	106.93	112.39
3	B	402	NAD	C5A-N7A-C8A	3.19	108.46	103.45
3	B	402	NAD	N9A-C8A-N7A	-3.16	109.45	113.94
3	B	402	NAD	C4D-O4D-C1D	-3.11	107.07	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	CAA	N9A-C8A-N7A	-3.08	109.57	113.94
3	B	402	NAD	C5N-C6N-N1N	-2.96	116.34	120.38
3	B	402	NAD	C2N-C3N-C7N	-2.94	110.99	119.46
2	B	401	CAA	C4A-C5A-N7A	-2.93	107.24	110.58
2	B	401	CAA	C5A-N7A-C8A	2.92	108.03	103.45
2	B	401	CAA	C3P-N4P-C5P	-2.71	117.78	122.82
2	B	401	CAA	O5B-C5B-C4B	-2.62	100.06	108.99
3	B	402	NAD	C4A-N9A-C8A	2.55	108.41	105.74
3	B	402	NAD	O7N-C7N-N7N	-2.50	119.00	122.62
2	B	401	CAA	CDP-CBP-CAP	2.41	112.87	108.77
2	B	401	CAA	O1-C1-S1P	-2.37	119.67	122.68
2	B	401	CAA	C4A-N9A-C8A	2.35	108.21	105.74
3	B	402	NAD	C3N-C7N-N7N	2.30	120.57	117.74
2	B	401	CAA	CEP-CBP-CCP	2.01	111.54	108.22

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	CAA	O4B-C1B-N9A-C4A
2	B	401	CAA	O4B-C1B-N9A-C8A
2	B	401	CAA	P2A-O3A-P1A-O5B
2	B	401	CAA	CCP-O6A-P2A-O3A
2	B	401	CAA	CCP-O6A-P2A-O4A
2	B	401	CAA	CCP-O6A-P2A-O5A
2	B	401	CAA	CAP-CBP-CCP-O6A
2	B	401	CAA	C1-C2-C3-O3
2	B	401	CAA	C1-C2-C3-C4
3	B	402	NAD	C5B-O5B-PA-O1A
3	B	402	NAD	C5B-O5B-PA-O2A
3	B	402	NAD	O4D-C1D-N1N-C2N
3	B	402	NAD	O4D-C1D-N1N-C6N
3	B	402	NAD	C2D-C1D-N1N-C6N
3	B	402	NAD	C4N-C3N-C7N-O7N
3	B	402	NAD	C4N-C3N-C7N-N7N
3	B	402	NAD	O4B-C4B-C5B-O5B
2	B	401	CAA	C3B-C4B-C5B-O5B
3	B	402	NAD	O4D-C4D-C5D-O5D
2	B	401	CAA	C4B-C5B-O5B-P1A
2	B	401	CAA	CDP-CBP-CCP-O6A
2	B	401	CAA	CEP-CBP-CCP-O6A
3	B	402	NAD	C2B-C1B-N9A-C8A

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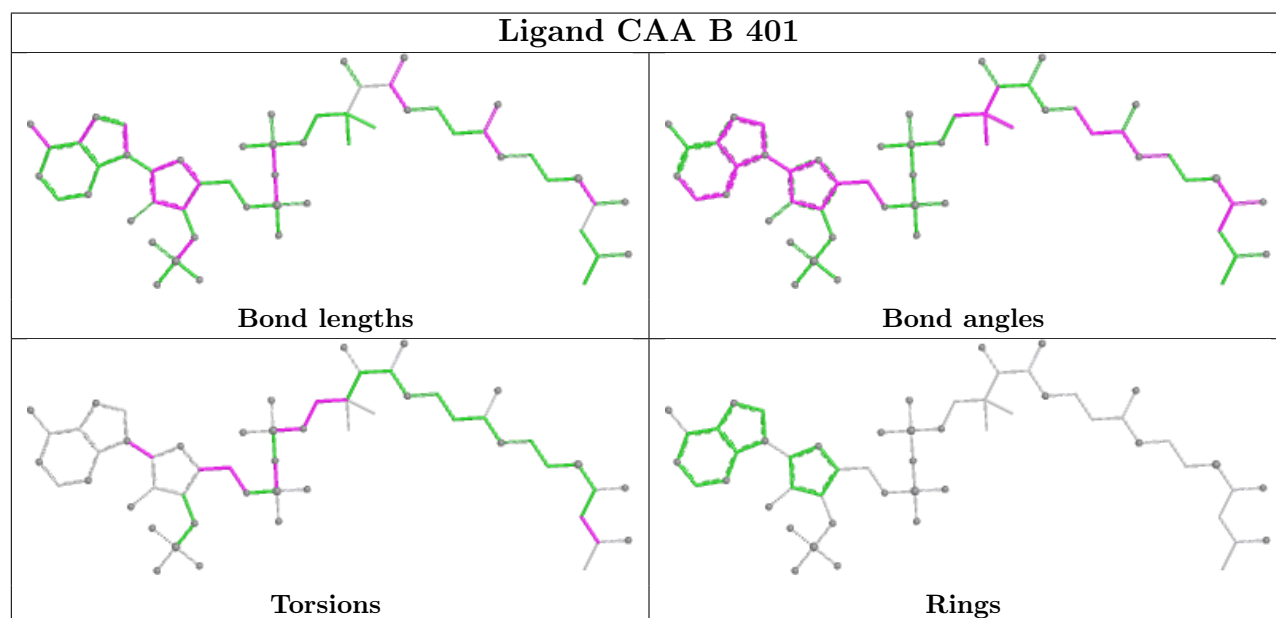
Mol	Chain	Res	Type	Atoms
3	B	402	NAD	C5B-O5B-PA-O3
2	B	401	CAA	CBP-CCP-O6A-P2A
3	B	402	NAD	C3D-C4D-C5D-O5D

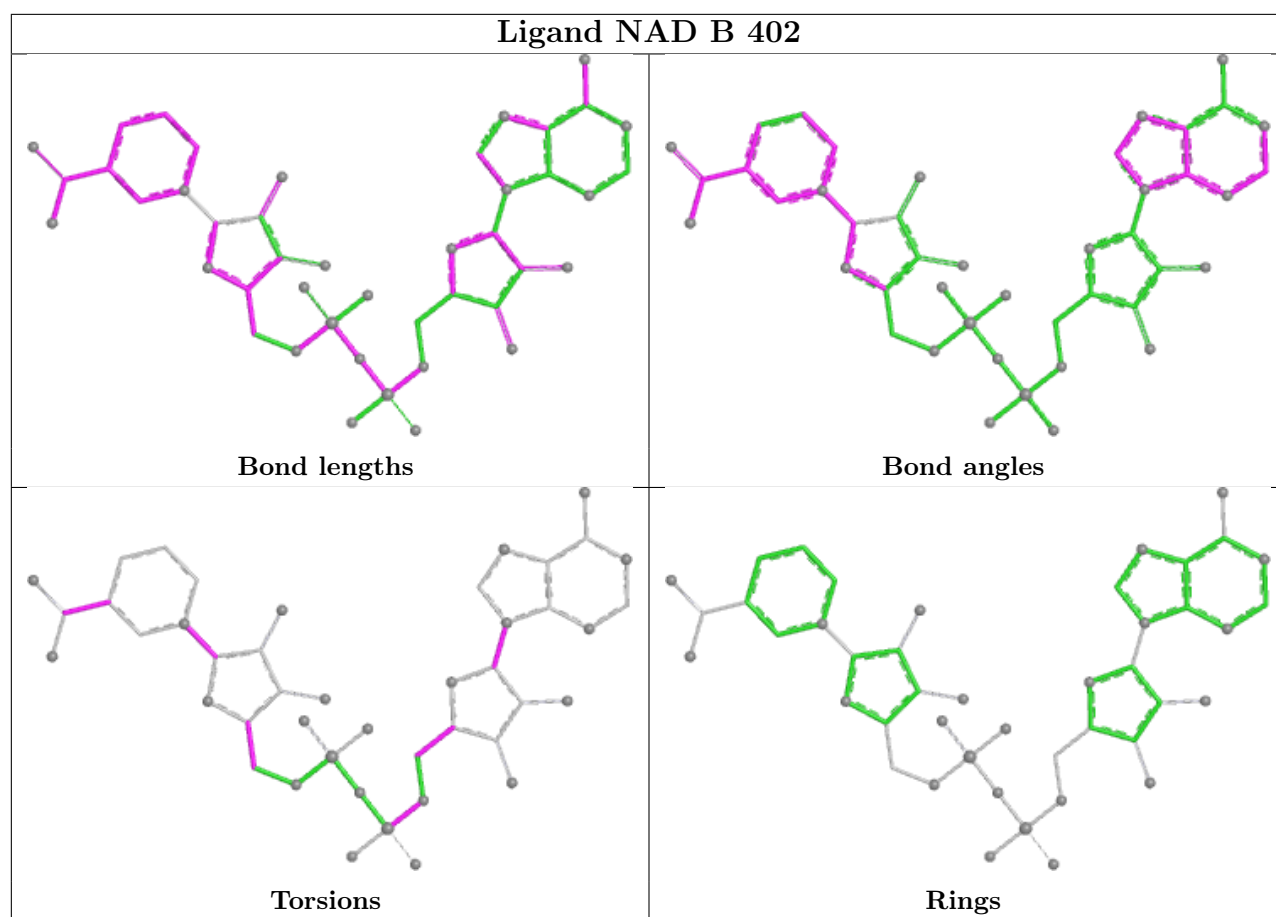
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	CAA	4	0
3	B	402	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	288/291 (98%)	-0.40	1 (0%) 90 88	20, 34, 55, 84	0
1	B	289/291 (99%)	0.09	17 (5%) 28 25	19, 38, 73, 93	0
1	C	290/291 (99%)	-0.43	0 100 100	21, 33, 51, 78	0
All	All	867/873 (99%)	-0.25	18 (2%) 63 60	19, 34, 64, 93	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	CYS	5.4
1	B	73	LEU	5.0
1	B	72	GLY	4.6
1	B	74	LYS	3.9
1	B	77	LEU	3.9
1	B	89	PHE	3.3
1	B	71	PRO	3.0
1	B	281	ASP	2.8
1	B	127	GLY	2.7
1	B	76	ASN	2.6
1	B	105	ILE	2.6
1	A	89	PHE	2.5
1	B	30	CYS	2.5
1	B	70	THR	2.4
1	B	106	CYS	2.2
1	B	36	TRP	2.2
1	B	31	ASP	2.1
1	B	8	ALA	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](#)

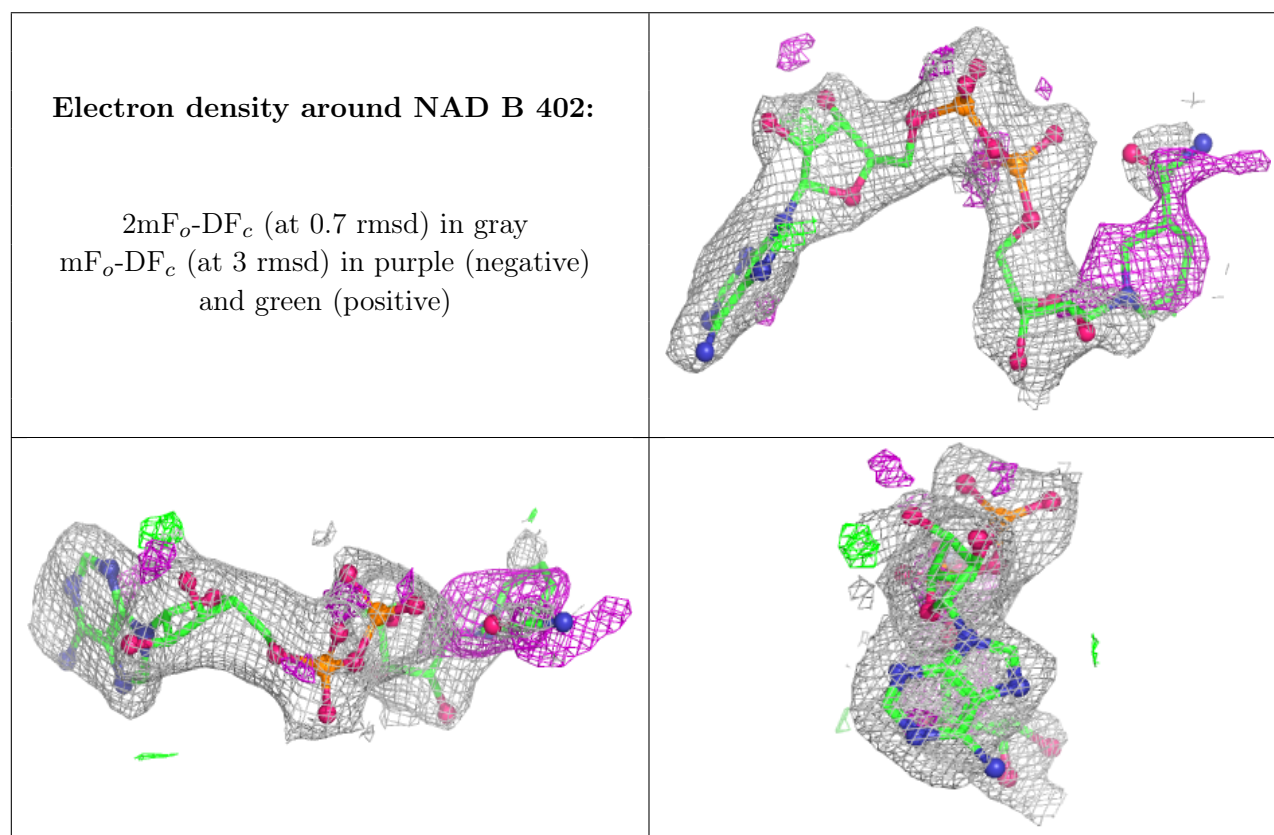
There are no oligosaccharides in this entry.

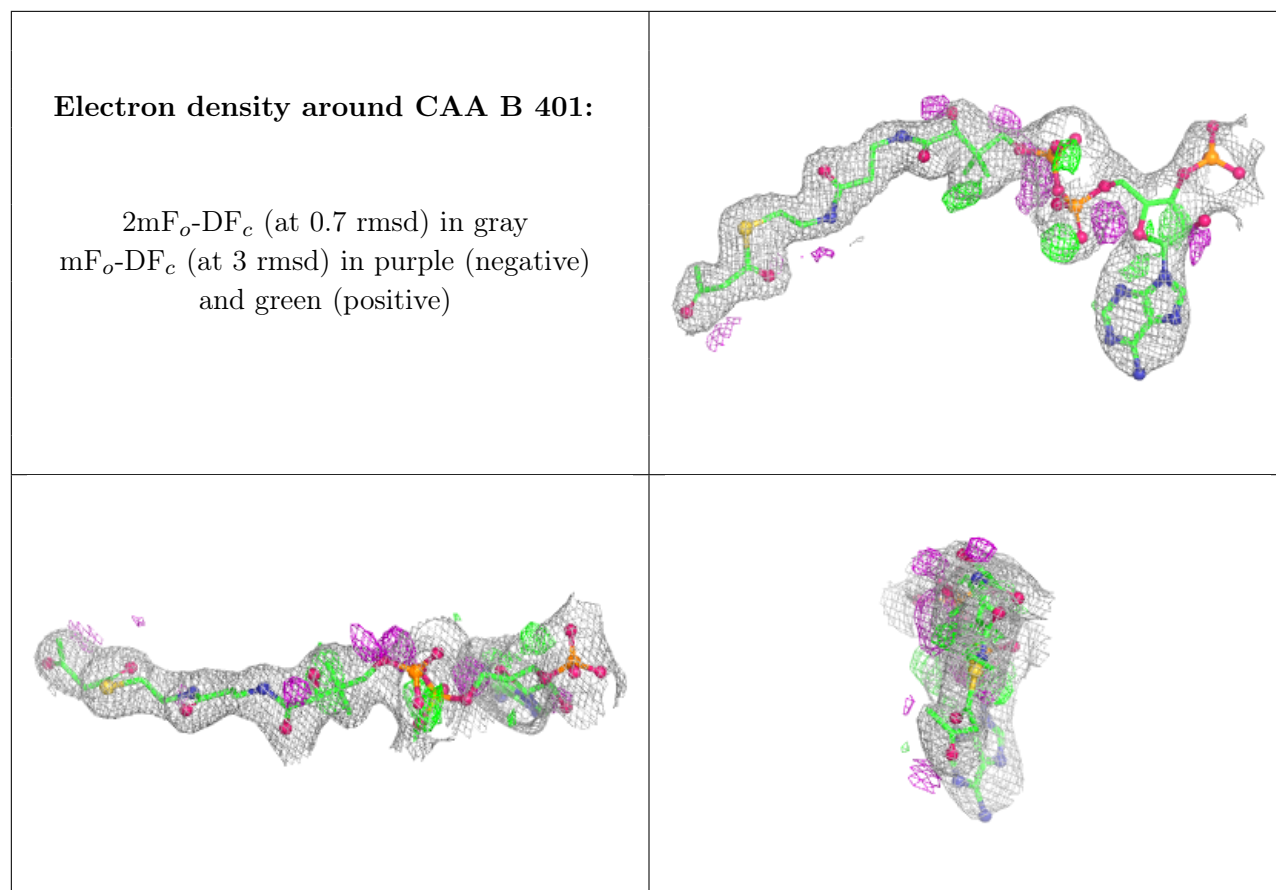
6.4 Ligands [i](#)

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
3	NAD	B	402	44/44	0.85	0.13	51,65,71,72	0
2	CAA	B	401	54/54	0.88	0.12	26,58,90,98	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 ⓘ

There are no such residues in this entry.