



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:23 PM UTC

PDB ID : 6TTB / pdb_00006ttb
Title : Crystal structure of NAD-dependent formate dehydrogenase from Staphylococcus aureus in complex with NAD
Authors : Boyko, K.M.; Pometun, A.A.; Nikolaeva, A.Y.; Kargov, I.S.; Yurchenko, T.S.; Savin, S.S.; Popov, V.O.; Tishkov, V.I.
Deposited on : 2019-12-26
Resolution : 2.70 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

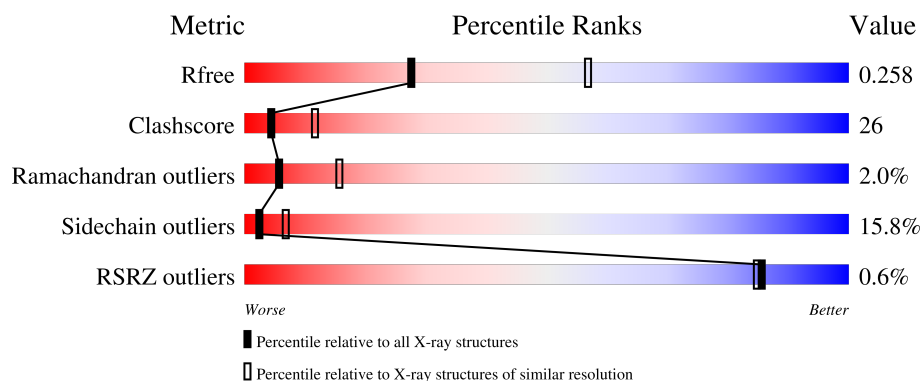
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	373	 47% 32% 10% 11%
1	B	373	 45% 34% 7% 12%

2 Entry composition [i](#)

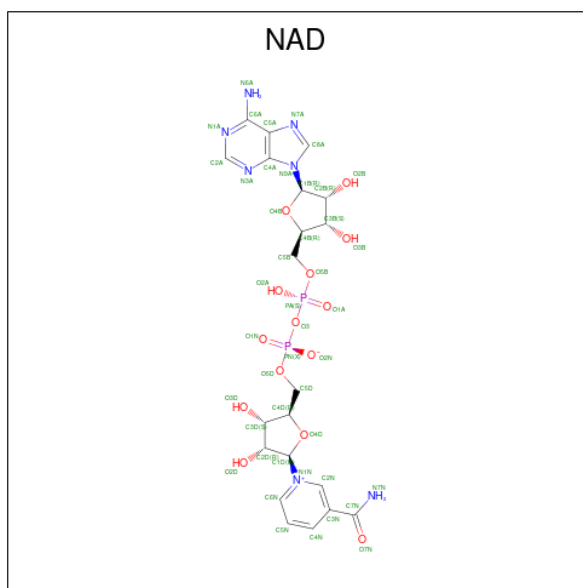
There are 3 unique types of molecules in this entry. The entry contains 5096 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Formate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2536	1609	444	475	8			
1	B	327	Total	C	N	O	S	0	0	0
			2504	1588	440	468	8			

- Molecule 2 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
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total	0	0
			5		

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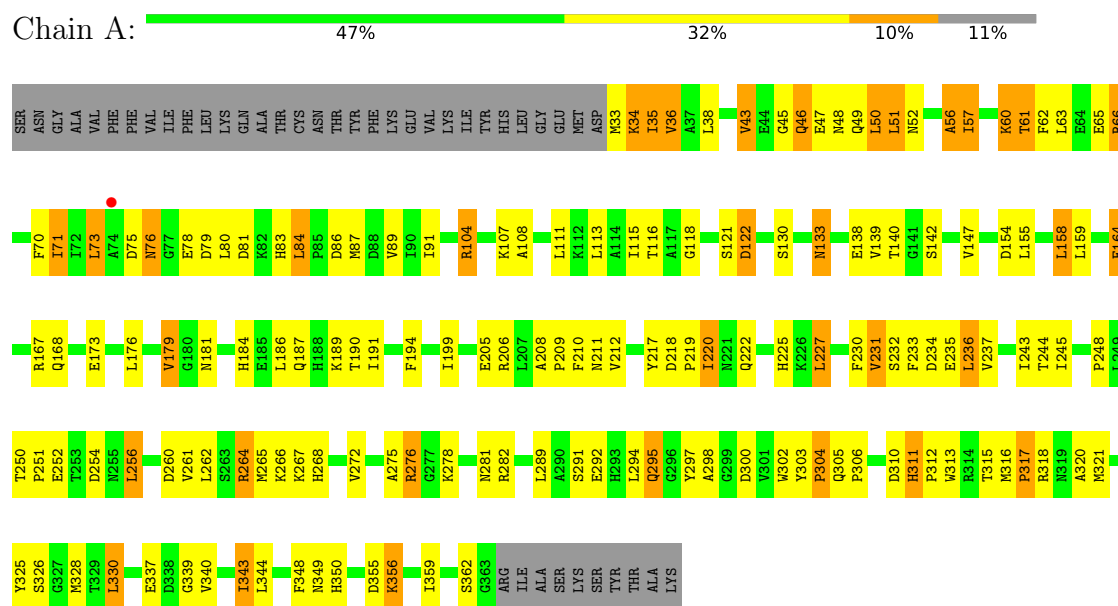
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	7	Total	O	0	0
			7	7		

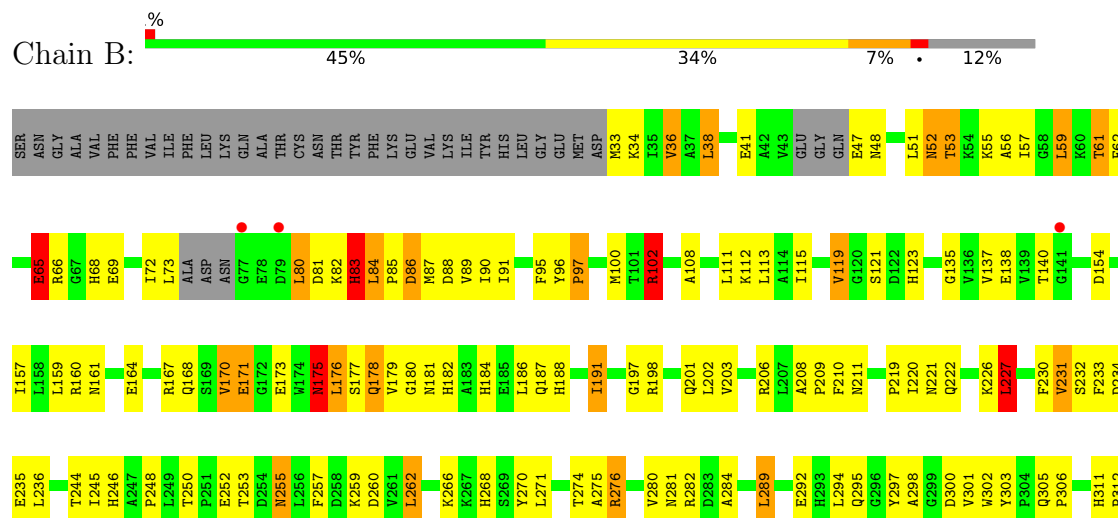
3 Residue-property plots [i](#)

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: Formate dehydrogenase



• Molecule 1: Formate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.29Å 87.36Å 117.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.70 – 2.70 59.70 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (59.70-2.70) 98.6 (59.70-2.70)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.182 , 0.257 0.183 , 0.258	Depositor DCC
R_{free} test set	1021 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.9	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	0.93	EDS
Total number of atoms	5096	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 5.08% 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

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	1.16	5/2594 (0.2%)	1.32	4/3533 (0.1%)
1	B	1.16	8/2560 (0.3%)	1.33	13/3488 (0.4%)
All	All	1.16	13/5154 (0.3%)	1.32	17/7021 (0.2%)

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	B	0	4
All	All	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	HIS	CE1-NE2	11.79	1.44	1.32
1	B	182	HIS	CE1-NE2	7.38	1.40	1.32
1	B	68	HIS	CE1-NE2	7.22	1.39	1.32
1	B	248	PRO	C-O	-6.93	1.15	1.23
1	A	121	SER	CA-CB	-6.76	1.43	1.53
1	B	268	HIS	CE1-NE2	6.35	1.38	1.32
1	B	178	GLN	C-O	-5.94	1.17	1.24
1	A	130	SER	CA-CB	-5.94	1.44	1.53
1	A	310	ASP	CG-OD2	5.91	1.36	1.25
1	B	184	HIS	CE1-NE2	5.78	1.38	1.32
1	B	121	SER	CA-CB	-5.64	1.45	1.53
1	A	256	LEU	C-O	-5.51	1.17	1.24
1	B	245	ILE	C-O	-5.36	1.18	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	ASN	CB-CA-C	11.89	126.74	111.40
1	B	244	THR	CB-CA-C	6.82	121.51	109.72
1	A	317	PRO	CB-CA-C	-6.72	100.47	111.56
1	B	220	ILE	CB-CA-C	6.63	116.95	111.05
1	B	102	ARG	CB-CG-CD	6.35	125.90	111.30
1	B	52	ASN	CB-CA-C	-6.21	98.80	110.16
1	B	244	THR	CA-CB-OG1	-5.93	100.71	109.60
1	B	274	THR	CB-CA-C	-5.87	101.51	111.02
1	A	133	ASN	CB-CA-C	5.79	119.95	111.73
1	B	65	GLU	CB-CA-C	5.67	119.56	110.09
1	A	220	ILE	CB-CA-C	5.57	116.65	111.30
1	B	112	LYS	N-CA-C	-5.46	107.27	114.31
1	B	253	THR	N-CA-C	-5.35	106.92	113.50
1	B	161	ASN	CA-CB-CG	5.33	117.92	112.60
1	B	219	PRO	CA-C-N	-5.30	117.55	123.16
1	B	219	PRO	C-N-CA	-5.30	117.55	123.16
1	A	122	ASP	CB-CA-C	5.04	120.05	110.27

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	73	LEU	Peptide
1	B	326	SER	Peptide
1	B	51	LEU	Peptide
1	B	80	LEU	Peptide
1	B	97	PRO	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	2536	0	2426	140	0
1	B	2504	0	2363	136	0
2	A	44	0	26	9	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	0	0	0	0
All	All	5096	0	4815	262	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 26.

All (262) 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:75:ASP:CB	1:A:79:ASP:HB3	1.61	1.27
1:B:102:ARG:HB2	1:B:102:ARG:HH11	0.95	1.11
1:B:102:ARG:HH11	1:B:102:ARG:CB	1.65	1.10
1:A:222:GLN:HG2	1:A:230:PHE:CE1	1.88	1.09
1:A:51:LEU:HD12	1:A:57:ILE:HD13	1.39	1.02
1:B:102:ARG:HB2	1:B:102:ARG:NH1	1.74	1.01
1:B:364:ARG:O	1:B:365:ILE:HB	1.58	1.00
1:A:57:ILE:HG13	1:A:337:GLU:HB2	1.44	0.98
1:B:33:MET:HA	1:B:88:ASP:OD2	1.65	0.96
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.31	0.94
1:B:41:GLU:HA	1:B:53:THR:OG1	1.69	0.91
1:A:222:GLN:HG2	1:A:230:PHE:CZ	2.06	0.91
1:B:81:ASP:O	1:B:84:LEU:HD13	1.78	0.83
1:A:71:ILE:HD12	1:A:83:HIS:CE1	2.15	0.81
1:A:46:GLN:NE2	1:B:178:GLN:HA	2.00	0.77
1:A:84:LEU:HD21	1:A:104:ARG:HG2	1.64	0.77
1:B:57:ILE:HG13	1:B:59:LEU:HD22	1.67	0.76
1:B:175:ASN:O	1:B:176:LEU:HB2	1.85	0.76
1:A:57:ILE:CG1	1:A:337:GLU:HB2	2.16	0.75
1:A:243:ILE:HD12	1:A:265:MET:HE3	1.68	0.75
1:A:48:ASN:HB2	1:B:181:ASN:OD1	1.87	0.75
1:B:34:LYS:HD3	1:B:87:MET:HA	1.69	0.75
1:A:46:GLN:HE22	1:B:178:GLN:HA	1.48	0.75
1:B:351:GLU:HB3	1:B:352:PRO:HD2	1.68	0.74
1:A:80:LEU:HD23	1:A:104:ARG:HE	1.53	0.74
1:A:61:THR:O	1:A:65:GLU:HB2	1.88	0.72
1:A:206:ARG:HG3	1:A:206:ARG:NH1	2.02	0.72
1:A:66:ARG:HG3	1:A:66:ARG:HH11	1.55	0.72
1:B:84:LEU:N	1:B:85:PRO:CD	2.53	0.71
1:B:61:THR:O	1:B:65:GLU:HB3	1.90	0.71
1:B:362:SER:H	1:B:365:ILE:HG22	1.56	0.71
1:A:168:GLN:NE2	1:A:179:VAL:HG22	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:SER:H	1:B:365:ILE:CG2	2.04	0.70
1:B:364:ARG:O	1:B:365:ILE:CB	2.34	0.69
1:A:138:GLU:CD	1:A:359:ILE:HD11	2.18	0.69
1:A:206:ARG:NH1	1:A:206:ARG:CG	2.56	0.68
1:A:233:PHE:O	1:A:234:ASP:C	2.36	0.67
1:B:222:GLN:HA	1:B:230:PHE:CD1	2.29	0.67
1:A:222:GLN:CG	1:A:230:PHE:CE1	2.74	0.67
1:A:248:PRO:HA	2:A:401:NAD:O3D	1.95	0.67
1:A:222:GLN:HA	1:A:230:PHE:CD1	2.30	0.67
1:A:75:ASP:CB	1:A:79:ASP:CB	2.57	0.66
1:A:80:LEU:HD23	1:A:104:ARG:NE	2.09	0.66
1:B:305:GLN:HA	1:B:306:PRO:C	2.21	0.66
1:A:305:GLN:HA	1:A:306:PRO:C	2.20	0.65
1:B:276:ARG:HG2	1:B:276:ARG:HH11	1.61	0.65
1:B:84:LEU:C	1:B:84:LEU:CD2	2.69	0.65
1:B:298:ALA:HB2	1:B:320:ALA:HB3	1.79	0.65
1:B:226:LYS:O	1:B:227:LEU:HB2	1.94	0.65
1:A:181:ASN:OD1	1:B:47:GLU:HA	1.97	0.65
1:B:95:PHE:CE2	1:B:328:MET:HE2	2.32	0.65
1:A:168:GLN:HE22	1:A:179:VAL:HG22	1.63	0.64
1:A:300:ASP:OD2	1:A:326:SER:HB3	1.97	0.64
1:B:325:TYR:O	1:B:326:SER:CB	2.45	0.64
1:A:315:THR:HG22	1:A:315:THR:O	1.98	0.63
1:A:138:GLU:OE1	1:A:359:ILE:HD11	1.98	0.63
1:A:81:ASP:HA	1:A:84:LEU:HD22	1.81	0.62
1:B:361:ALA:HA	1:B:365:ILE:HG21	1.82	0.62
1:A:66:ARG:HH11	1:A:66:ARG:CG	2.11	0.62
1:A:139:VAL:HG12	1:A:142:SER:HB3	1.81	0.62
1:B:81:ASP:HA	1:B:84:LEU:HD12	1.82	0.61
1:A:87:MET:HE3	1:A:111:LEU:HD13	1.83	0.61
1:A:217:TYR:CD1	1:A:217:TYR:C	2.78	0.61
1:B:81:ASP:HA	1:B:84:LEU:CD1	2.30	0.60
1:A:51:LEU:CD1	1:A:57:ILE:HD13	2.23	0.60
1:A:167:ARG:HH22	1:A:173:GLU:CD	2.09	0.60
1:B:90:ILE:HG13	1:B:91:ILE:N	2.16	0.60
1:B:95:PHE:CE2	1:B:328:MET:CE	2.85	0.60
1:B:62:PHE:O	1:B:66:ARG:NH1	2.35	0.59
1:B:52:ASN:HB3	1:B:55:LYS:H	1.67	0.59
1:B:177:SER:O	1:B:181:ASN:HB2	2.02	0.59
1:B:233:PHE:O	1:B:234:ASP:C	2.46	0.58
1:B:72:ILE:C	1:B:73:LEU:HD23	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ILE:O	1:B:73:LEU:HD23	2.03	0.58
1:A:208:ALA:N	1:A:209:PRO:CD	2.67	0.57
1:B:167:ARG:O	1:B:171:GLU:HB2	2.04	0.57
1:A:209:PRO:HG2	1:B:209:PRO:HG3	1.85	0.57
1:B:187:GLN:HG3	1:B:211:ASN:HB3	1.86	0.57
1:B:84:LEU:O	1:B:108:ALA:HA	2.05	0.57
1:B:87:MET:HE3	1:B:111:LEU:HD22	1.86	0.57
1:A:46:GLN:HE22	1:B:178:GLN:CA	2.18	0.57
1:B:62:PHE:CD2	1:B:341:LYS:HD3	2.39	0.57
1:B:90:ILE:HG12	1:B:100:MET:HE3	1.86	0.57
1:B:137:VAL:HG12	1:B:138:GLU:N	2.20	0.57
1:A:46:GLN:NE2	1:B:178:GLN:CA	2.68	0.57
1:B:255:ASN:HD21	1:B:281:ASN:HD22	1.53	0.57
1:B:326:SER:C	1:B:328:MET:H	2.13	0.56
1:A:206:ARG:HD3	1:B:210:PHE:CE1	2.41	0.56
1:A:43:VAL:HB	1:A:46:GLN:CG	2.35	0.56
1:A:218:ASP:OD1	2:A:401:NAD:O2B	2.21	0.55
1:A:34:LYS:HD3	1:A:87:MET:HA	1.88	0.55
1:B:137:VAL:HG13	1:B:357:ASP:O	2.06	0.55
1:A:38:LEU:HD12	1:A:73:LEU:O	2.05	0.55
1:A:164:GLU:OE2	1:A:167:ARG:HD3	2.06	0.55
1:B:300:ASP:O	1:B:324:HIS:HB2	2.07	0.55
1:A:45:GLY:O	1:A:47:GLU:N	2.39	0.55
1:B:311:HIS:ND1	1:B:312:PRO:HD2	2.21	0.55
1:B:38:LEU:CD2	1:B:96:TYR:HE1	2.20	0.54
1:A:295:GLN:OE1	1:A:295:GLN:HA	2.07	0.54
1:B:119:VAL:HG12	1:B:119:VAL:O	2.05	0.54
1:A:218:ASP:CG	2:A:401:NAD:HO2A	2.16	0.54
1:A:325:TYR:HB2	1:A:328:MET:HE2	1.88	0.54
1:B:326:SER:H	1:B:328:MET:H	1.54	0.54
1:A:147:VAL:HG21	2:A:401:NAD:C4N	2.39	0.53
1:B:137:VAL:CG1	1:B:138:GLU:N	2.71	0.53
1:B:168:GLN:NE2	1:B:175:ASN:HB2	2.23	0.53
1:B:175:ASN:O	1:B:176:LEU:CB	2.57	0.53
1:B:354:GLN:HG2	1:B:356:LYS:HE2	1.91	0.53
1:A:199:ILE:HD12	2:A:401:NAD:H51N	1.90	0.52
1:B:175:ASN:OD1	1:B:178:GLN:HB2	2.10	0.52
1:B:84:LEU:HB2	1:B:87:MET:HE2	1.91	0.52
1:A:302:TRP:HB2	1:A:305:GLN:HG2	1.91	0.52
1:B:84:LEU:N	1:B:85:PRO:HD2	2.22	0.52
1:A:291:SER:C	1:A:292:GLU:HG3	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LEU:O	1:A:108:ALA:HA	2.11	0.51
1:A:300:ASP:OD2	1:A:326:SER:CB	2.59	0.51
1:B:48:ASN:C	1:B:48:ASN:OD1	2.53	0.51
1:B:164:GLU:OE2	1:B:178:GLN:HG2	2.09	0.51
1:B:270:TYR:CE1	1:B:295:GLN:HB3	2.46	0.51
1:B:84:LEU:C	1:B:84:LEU:HD22	2.35	0.50
1:B:187:GLN:O	1:B:188:HIS:HB2	2.12	0.50
1:B:326:SER:C	1:B:328:MET:N	2.70	0.50
1:A:260:ASP:O	1:A:264:ARG:HG3	2.11	0.50
1:B:81:ASP:O	1:B:83:HIS:N	2.41	0.50
1:A:159:LEU:HD13	1:A:186:LEU:HD13	1.93	0.50
1:A:190:THR:C	1:A:191:ILE:HD13	2.37	0.50
1:A:50:LEU:HB3	1:A:57:ILE:HD12	1.93	0.50
1:A:80:LEU:CD2	1:A:104:ARG:HE	2.24	0.50
1:B:170:VAL:HG12	1:B:171:GLU:OE2	2.12	0.50
1:A:205:GLU:HA	1:A:227:LEU:CD2	2.41	0.50
1:A:133:ASN:HD21	1:A:362:SER:HA	1.76	0.50
1:B:33:MET:HG3	1:B:348:PHE:HE1	1.76	0.49
1:B:73:LEU:HD13	1:B:80:LEU:CB	2.42	0.49
1:B:186:LEU:HD11	1:B:191:ILE:HD11	1.95	0.49
1:A:48:ASN:HB2	1:B:181:ASN:CG	2.38	0.49
1:A:62:PHE:O	1:A:66:ARG:HG3	2.12	0.49
1:B:362:SER:N	1:B:365:ILE:HG21	2.27	0.49
1:B:175:ASN:HB3	1:B:176:LEU:H	1.42	0.49
1:A:256:LEU:O	1:A:261:VAL:HG21	2.13	0.48
1:B:301:VAL:HA	1:B:305:GLN:OE1	2.13	0.48
1:A:315:THR:O	1:A:315:THR:CG2	2.60	0.48
1:B:154:ASP:HB3	1:B:298:ALA:HB3	1.94	0.48
1:A:199:ILE:HD12	2:A:401:NAD:C5D	2.44	0.48
1:A:267:LYS:O	1:A:268:HIS:HB2	2.14	0.48
1:A:43:VAL:HB	1:A:46:GLN:HG3	1.94	0.48
1:A:298:ALA:HB2	1:A:320:ALA:HB3	1.96	0.48
1:B:86:ASP:OD1	1:B:86:ASP:N	2.46	0.48
1:B:362:SER:N	1:B:365:ILE:CG2	2.76	0.48
1:A:313:TRP:HA	1:A:316:MET:SD	2.54	0.48
1:B:326:SER:H	1:B:328:MET:N	2.11	0.48
1:A:91:ILE:HG12	1:A:115:ILE:HB	1.96	0.47
1:B:197:GLY:O	1:B:201:GLN:HB2	2.14	0.47
1:A:254:ASP:OD1	1:A:278:LYS:HD3	2.14	0.47
1:A:36:VAL:HG23	1:A:87:MET:HB2	1.96	0.47
1:B:334:LYS:O	1:B:337:GLU:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:O	1:A:222:GLN:HG3	2.14	0.47
1:A:57:ILE:HG23	1:A:57:ILE:O	2.13	0.47
1:B:164:GLU:OE1	1:B:164:GLU:HA	2.15	0.47
1:B:168:GLN:HE21	1:B:178:GLN:HG2	1.80	0.47
1:A:167:ARG:NH2	1:A:173:GLU:CD	2.73	0.47
1:B:84:LEU:C	1:B:84:LEU:HD23	2.38	0.47
1:B:208:ALA:N	1:B:209:PRO:CD	2.78	0.47
1:B:275:ALA:C	1:B:276:ARG:HG2	2.40	0.47
1:B:362:SER:O	1:B:364:ARG:N	2.48	0.47
1:B:302:TRP:HB2	1:B:305:GLN:HG3	1.97	0.47
1:B:66:ARG:HG3	1:B:66:ARG:HH11	1.79	0.47
1:A:261:VAL:O	1:A:262:LEU:C	2.55	0.46
1:A:250:THR:HB	1:A:251:PRO:CD	2.46	0.46
1:A:205:GLU:HA	1:A:227:LEU:HD21	1.97	0.46
1:B:89:VAL:HG22	1:B:113:LEU:HB3	1.97	0.46
1:B:102:ARG:CB	1:B:102:ARG:NH1	2.51	0.46
1:A:311:HIS:ND1	1:A:312:PRO:HD2	2.31	0.46
1:B:56:ALA:C	1:B:57:ILE:HG12	2.40	0.46
1:A:159:LEU:HD13	1:A:186:LEU:CD1	2.45	0.46
1:A:275:ALA:C	1:A:276:ARG:HG2	2.40	0.46
1:A:303:TYR:HA	1:A:304:PRO:HA	1.79	0.45
1:B:235:GLU:O	1:B:236:LEU:C	2.58	0.45
1:B:36:VAL:CG2	1:B:87:MET:HB2	2.47	0.45
1:B:179:VAL:HG13	1:B:180:GLY:N	2.32	0.45
1:B:257:PHE:HB2	1:B:280:VAL:HG22	1.97	0.45
1:A:209:PRO:CG	1:B:209:PRO:HG3	2.47	0.45
1:A:60:LYS:HB2	1:A:60:LYS:HE2	1.21	0.44
1:A:115:ILE:CD1	1:A:344:LEU:HD21	2.48	0.44
1:B:337:GLU:O	1:B:341:LYS:HG3	2.18	0.44
1:A:231:VAL:HG13	1:A:232:SER:O	2.18	0.44
1:A:330:LEU:HD12	1:A:330:LEU:HA	1.75	0.44
1:A:86:ASP:N	1:A:86:ASP:OD1	2.51	0.44
1:A:343:ILE:HG22	1:A:344:LEU:N	2.33	0.44
1:A:225:HIS:CE1	1:A:227:LEU:HB2	2.52	0.44
1:A:328:MET:O	1:A:328:MET:HG2	2.18	0.44
1:A:159:LEU:CD1	1:A:186:LEU:HD13	2.47	0.44
1:A:291:SER:C	1:A:292:GLU:CG	2.90	0.44
1:B:157:ILE:O	1:B:160:ARG:O	2.36	0.44
1:B:271:LEU:HB3	1:B:297:TYR:HD1	1.83	0.43
1:A:344:LEU:O	1:A:348:PHE:CD2	2.72	0.43
1:B:226:LYS:O	1:B:227:LEU:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:GLU:HB3	1:B:352:PRO:CD	2.42	0.43
1:A:168:GLN:HG2	1:A:173:GLU:OE2	2.19	0.43
1:B:59:LEU:HD12	1:B:59:LEU:HA	1.89	0.43
1:B:90:ILE:HG21	1:B:100:MET:HE3	2.01	0.43
1:B:175:ASN:CB	1:B:178:GLN:HB3	2.49	0.43
1:A:139:VAL:O	1:A:140:THR:C	2.61	0.43
1:A:349:ASN:O	1:A:350:HIS:C	2.62	0.43
1:B:36:VAL:HG23	1:B:87:MET:HB2	2.01	0.43
1:A:187:GLN:HG3	1:A:211:ASN:HB3	2.01	0.43
1:B:102:ARG:HH11	1:B:102:ARG:CG	2.27	0.43
1:B:231:VAL:HG13	1:B:232:SER:O	2.19	0.43
1:A:115:ILE:HD11	1:A:344:LEU:CD2	2.49	0.43
1:A:167:ARG:NH2	1:A:173:GLU:OE2	2.47	0.43
1:B:281:ASN:O	1:B:282:ARG:C	2.62	0.43
1:A:219:PRO:O	1:A:222:GLN:CD	2.61	0.43
1:A:330:LEU:HD13	1:B:180:GLY:O	2.17	0.43
1:B:38:LEU:CD2	1:B:96:TYR:CE1	3.00	0.43
1:B:135:GLY:HA3	1:B:365:ILE:HD13	2.01	0.43
1:A:237:VAL:O	1:A:265:MET:HA	2.19	0.42
1:A:276:ARG:HE	2:A:401:NAD:HO2N	1.66	0.42
1:A:49:GLN:HB3	1:A:52:ASN:ND2	2.34	0.42
1:A:281:ASN:O	1:A:282:ARG:C	2.62	0.42
1:A:355:ASP:O	1:A:356:LYS:C	2.62	0.42
1:A:49:GLN:HB3	1:A:52:ASN:HD22	1.83	0.42
1:B:203:VAL:HG21	1:B:246:HIS:CE1	2.54	0.42
1:B:305:GLN:CA	1:B:306:PRO:C	2.92	0.42
1:A:219:PRO:HG2	2:A:401:NAD:HO2A	1.85	0.42
1:B:330:LEU:HD12	1:B:330:LEU:HA	1.88	0.42
1:A:116:THR:O	1:A:118:GLY:N	2.53	0.42
1:A:244:THR:HA	1:A:272:VAL:O	2.19	0.42
1:B:259:LYS:O	1:B:259:LYS:HG3	2.19	0.42
1:A:154:ASP:O	1:A:158:LEU:HB2	2.20	0.42
1:B:175:ASN:HB3	1:B:178:GLN:HB3	2.02	0.42
1:B:281:ASN:HB3	1:B:284:ALA:HB3	2.01	0.42
1:A:84:LEU:HD12	1:A:84:LEU:HA	1.84	0.42
1:A:34:LYS:C	1:A:35:ILE:HD12	2.44	0.42
1:A:340:VAL:O	1:A:344:LEU:HG	2.20	0.41
1:B:33:MET:HG3	1:B:348:PHE:CE1	2.54	0.41
1:A:60:LYS:HA	1:A:70:PHE:CD2	2.55	0.41
1:A:63:LEU:C	1:A:65:GLU:H	2.27	0.41
1:A:158:LEU:HD21	1:A:298:ALA:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:VAL:HG22	1:A:113:LEU:HB3	2.02	0.41
1:A:168:GLN:HA	1:A:173:GLU:HB2	2.03	0.41
1:B:255:ASN:HD21	1:B:281:ASN:ND2	2.16	0.41
1:B:275:ALA:O	1:B:276:ARG:HG2	2.21	0.41
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.84	0.41
1:B:289:LEU:O	1:B:292:GLU:N	2.50	0.41
1:A:52:ASN:O	1:A:56:ALA:HA	2.20	0.41
1:A:208:ALA:HB3	1:A:209:PRO:HD3	2.01	0.41
1:B:262:LEU:HD12	1:B:262:LEU:HA	1.82	0.41
1:A:84:LEU:HD21	1:A:104:ARG:CG	2.45	0.41
1:A:86:ASP:O	1:A:87:MET:C	2.61	0.41
1:A:184:HIS:HA	1:B:331:GLU:OE1	2.21	0.41
1:A:194:PHE:CE1	2:A:401:NAD:H2A	2.55	0.41
1:A:210:PHE:CE1	1:B:206:ARG:HG2	2.55	0.41
1:A:339:GLY:O	1:A:340:VAL:C	2.64	0.41
1:B:97:PRO:HB3	1:B:123:HIS:CG	2.56	0.41
1:B:344:LEU:O	1:B:348:PHE:CD2	2.73	0.41
1:A:43:VAL:HG23	1:B:177:SER:HB2	2.03	0.40
1:B:282:ARG:NH2	1:B:303:TYR:O	2.54	0.40
1:B:301:VAL:C	1:B:302:TRP:CD1	2.99	0.40
1:A:62:PHE:CD1	1:A:62:PHE:C	2.99	0.40
1:A:297:TYR:HE1	1:A:321:MET:SD	2.44	0.40
1:B:208:ALA:N	1:B:209:PRO:HD2	2.36	0.40
1:A:235:GLU:O	1:A:236:LEU:C	2.64	0.40
1:A:225:HIS:ND1	1:A:227:LEU:N	2.70	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	329/373 (88%)	291 (88%)	33 (10%)	5 (2%)	8 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	321/373 (86%)	282 (88%)	31 (10%)	8 (2%)	4	11
All	All	650/746 (87%)	573 (88%)	64 (10%)	13 (2%)	6	16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	ASN
1	B	176	LEU
1	B	227	LEU
1	A	78	GLU
1	A	356	LYS
1	B	82	LYS
1	B	83	HIS
1	B	326	SER
1	B	363	GLY
1	A	76	ASN
1	A	317	PRO
1	A	56	ALA
1	B	86	ASP

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	260/317 (82%)	219 (84%)	41 (16%)	2	7
1	B	252/317 (80%)	212 (84%)	40 (16%)	2	7
All	All	512/634 (81%)	431 (84%)	81 (16%)	2	7

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	MET
1	A	34	LYS
1	A	35	ILE

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Mol	Chain	Res	Type
1	A	36	VAL
1	A	43	VAL
1	A	46	GLN
1	A	50	LEU
1	A	51	LEU
1	A	57	ILE
1	A	60	LYS
1	A	61	THR
1	A	66	ARG
1	A	71	ILE
1	A	76	ASN
1	A	84	LEU
1	A	104	ARG
1	A	107	LYS
1	A	122	ASP
1	A	155	LEU
1	A	158	LEU
1	A	164	GLU
1	A	176	LEU
1	A	179	VAL
1	A	189	LYS
1	A	212	VAL
1	A	220	ILE
1	A	227	LEU
1	A	231	VAL
1	A	236	LEU
1	A	245	ILE
1	A	252	GLU
1	A	264	ARG
1	A	266	LYS
1	A	276	ARG
1	A	289	LEU
1	A	294	LEU
1	A	295	GLN
1	A	304	PRO
1	A	318	ARG
1	A	330	LEU
1	A	343	ILE
1	B	36	VAL
1	B	38	LEU
1	B	53	THR
1	B	59	LEU

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Mol	Chain	Res	Type
1	B	61	THR
1	B	65	GLU
1	B	69	GLU
1	B	83	HIS
1	B	84	LEU
1	B	102	ARG
1	B	115	ILE
1	B	119	VAL
1	B	140	THR
1	B	159	LEU
1	B	170	VAL
1	B	171	GLU
1	B	173	GLU
1	B	175	ASN
1	B	191	ILE
1	B	198	ARG
1	B	202	LEU
1	B	221	ASN
1	B	227	LEU
1	B	231	VAL
1	B	250	THR
1	B	252	GLU
1	B	255	ASN
1	B	260	ASP
1	B	262	LEU
1	B	266	LYS
1	B	276	ARG
1	B	289	LEU
1	B	294	LEU
1	B	315	THR
1	B	328	MET
1	B	330	LEU
1	B	331	GLU
1	B	354	GLN
1	B	356	LYS
1	B	365	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	133	ASN

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Mol	Chain	Res	Type
1	A	188	HIS
1	A	211	ASN
1	A	295	GLN
1	A	350	HIS
1	B	68	HIS
1	B	83	HIS
1	B	133	ASN
1	B	168	GLN
1	B	187	GLN
1	B	211	ASN
1	B	255	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	A	401	-	46,48,48	1.55	4 (8%)	64,73,73	0.81	1 (1%)

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	401	-	-	11/30/62/62	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAD	C2N-N1N	7.60	1.43	1.35
2	A	401	NAD	C4N-C3N	3.58	1.44	1.39
2	A	401	NAD	PA-O3	-3.13	1.56	1.59
2	A	401	NAD	PN-O3	-2.71	1.56	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAD	C6N-N1N-C2N	-2.23	119.98	121.88

There are no chirality outliers.

All (11) torsion outliers are listed below:

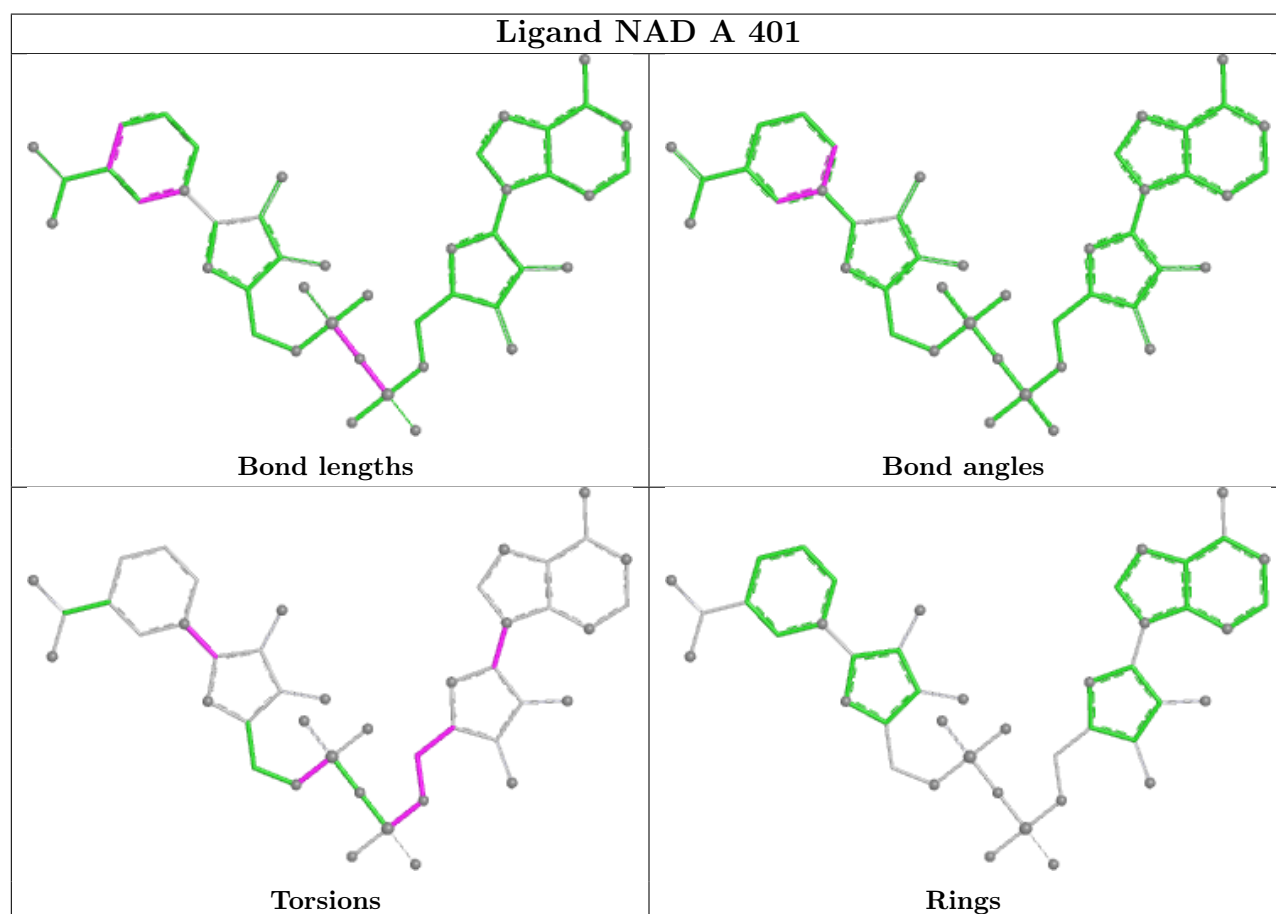
Mol	Chain	Res	Type	Atoms
2	A	401	NAD	C5B-O5B-PA-O1A
2	A	401	NAD	O4D-C1D-N1N-C6N
2	A	401	NAD	O4B-C4B-C5B-O5B
2	A	401	NAD	C3B-C4B-C5B-O5B
2	A	401	NAD	C2B-C1B-N9A-C8A
2	A	401	NAD	C5B-O5B-PA-O3
2	A	401	NAD	C5D-O5D-PN-O2N
2	A	401	NAD	C2D-C1D-N1N-C6N
2	A	401	NAD	O4D-C1D-N1N-C2N
2	A	401	NAD	C4B-C5B-O5B-PA
2	A	401	NAD	O4B-C1B-N9A-C8A

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAD	9	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	331/373 (88%)	-0.48	1 (0%) 90 89	10, 24, 41, 76	0
1	B	327/373 (87%)	-0.31	3 (0%) 81 80	12, 28, 53, 101	0
All	All	658/746 (88%)	-0.40	4 (0%) 85 85	10, 26, 50, 101	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	141	GLY	4.2
1	B	79	ASP	2.9
1	B	77	GLY	2.5
1	A	74	ALA	2.5

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](#)

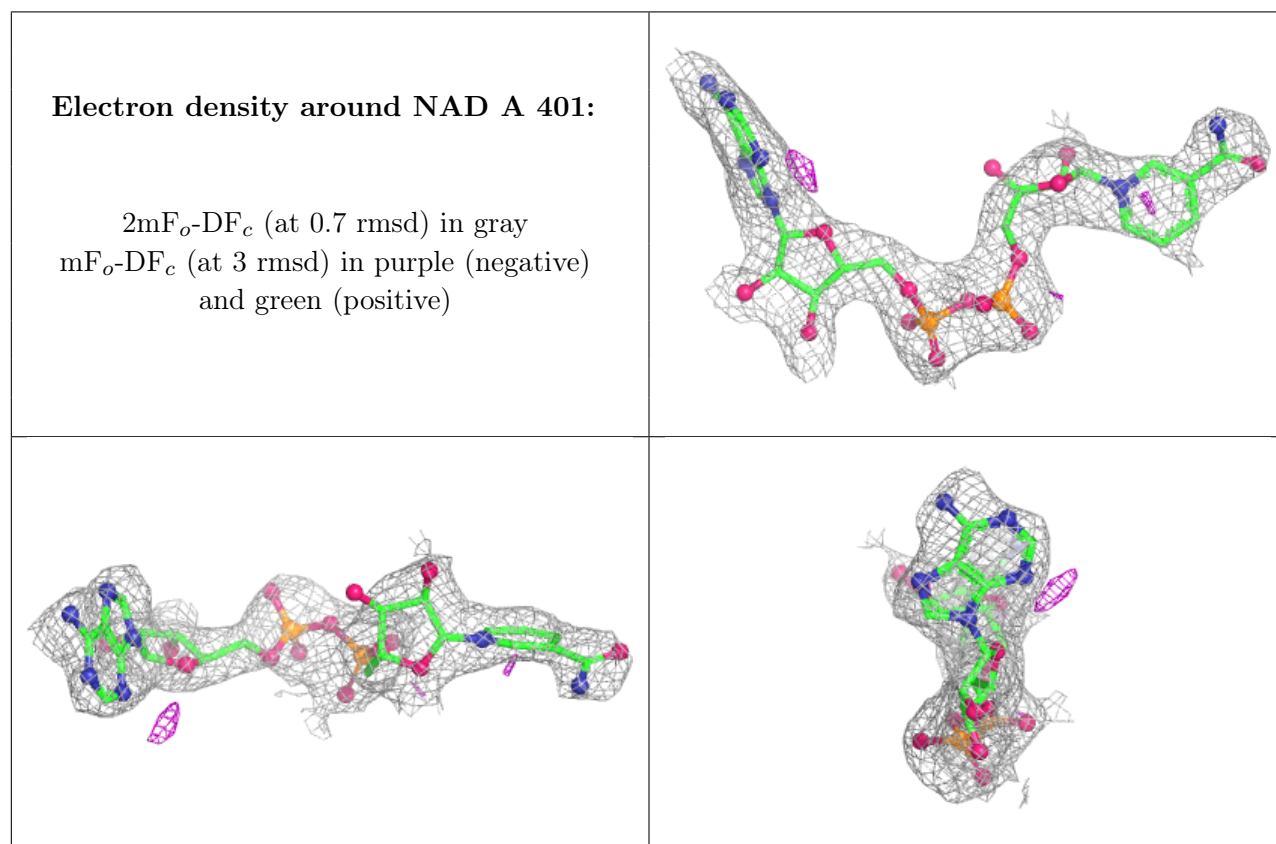
There are no oligosaccharides in this entry.

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
2	NAD	A	401	44/44	0.93	0.10	33,47,58,70	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.