Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 10:02 AM GMT

PDB ID	:	6TTB
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 following versions of software and data (see references ⓘ) were used in the production of this report:

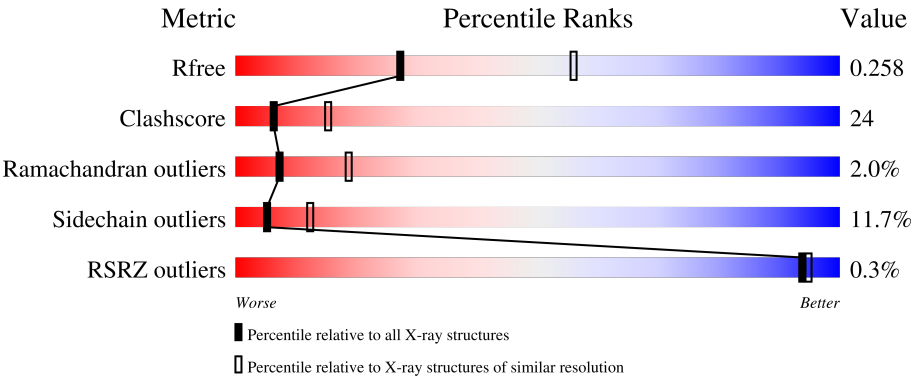
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	51% 32% 6% 11%
1	B	373	% 50% 30% 7% • 12%

2 Entry composition

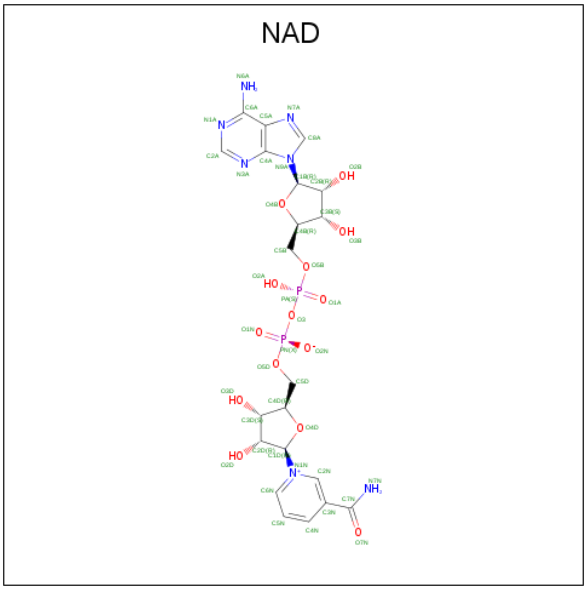
There are 3 unique types of molecules in this entry. The entry contains 5096 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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	O	0	0
			5	5		

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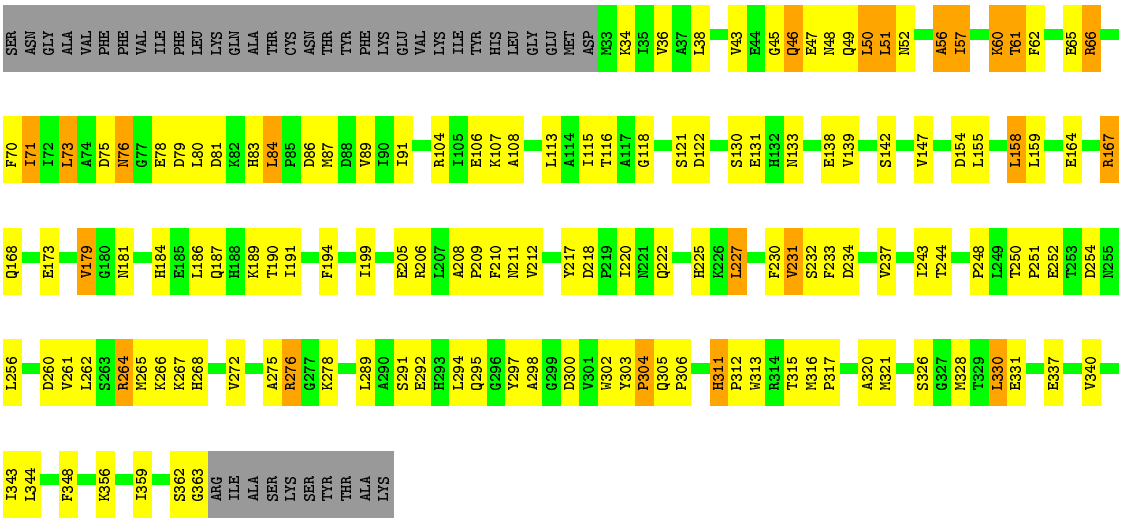
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	7	Total O 7 7	0	0

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.

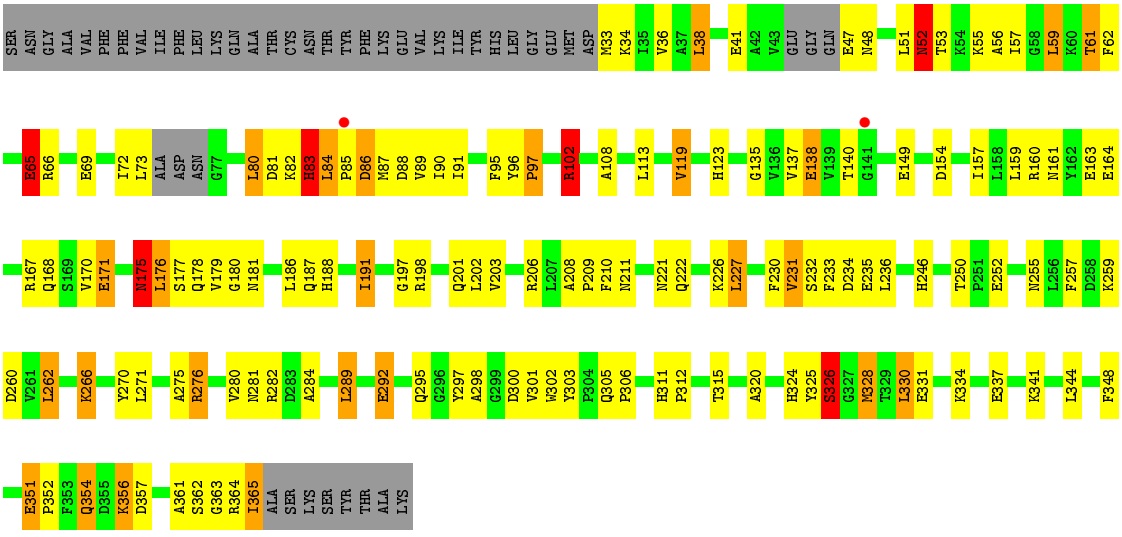
- Molecule 1: Formate dehydrogenase

Chain A:



- Molecule 1: Formate dehydrogenase

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.12%)	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)	0.41 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.88	7/2594 (0.3%)	0.94	1/3533 (0.0%)
1	B	0.85	6/2560 (0.2%)	0.92	5/3488 (0.1%)
All	All	0.87	13/5154 (0.3%)	0.93	6/7021 (0.1%)

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	106	GLU	CD-OE2	7.41	1.33	1.25
1	B	149	GLU	CD-OE1	7.05	1.33	1.25
1	B	351	GLU	CD-OE1	6.19	1.32	1.25
1	A	121	SER	CA-CB	-6.05	1.43	1.52
1	B	292	GLU	CD-OE1	5.98	1.32	1.25
1	A	130	SER	CA-CB	-5.87	1.44	1.52
1	A	331	GLU	CD-OE1	5.70	1.31	1.25
1	A	131	GLU	CD-OE2	5.67	1.31	1.25
1	B	65	GLU	CD-OE1	5.37	1.31	1.25
1	B	163	GLU	CD-OE1	5.21	1.31	1.25
1	B	138	GLU	CD-OE1	5.20	1.31	1.25
1	A	363	GLY	C-O	5.13	1.31	1.23
1	A	311	HIS	CE1-NE2	5.08	1.44	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	161	ASN	CB-CA-C	8.17	126.74	110.40
1	B	52	ASN	CB-CA-C	-5.80	98.80	110.40
1	B	102	ARG	CB-CG-CD	5.50	125.90	111.60
1	B	266	LYS	CB-CA-C	-5.30	99.79	110.40
1	B	102	ARG	CG-CD-NE	5.15	122.62	111.80
1	A	167	ARG	CG-CD-NE	-5.09	101.10	111.80

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 (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	2536	0	2426	124	0
1	B	2504	0	2363	130	0
2	A	44	0	26	7	0
3	A	5	0	0	0	0
3	B	7	0	0	0	0
All	All	5096	0	4815	240	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 24.

All (240) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ARG:HB2	1:B:102:ARG:HH11	0.95	1.11
1:B:102:ARG:CB	1:B:102:ARG:HH11	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:NH1	1:B:102:ARG:HB2	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: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:NH1	1:A:206:ARG:HG3	2.02	0.72
1:A:66:ARG:HH11	1:A:66:ARG:HG3	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
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:206:ARG:NH1	1:A:206:ARG:CG	2.56	0.68
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:276:ARG:HH11	1:B:276:ARG:HG2	1.61	0.65
1:B:298:ALA:HB2	1:B:320:ALA:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:138:GLU:CD	1:A:359:ILE:HD11	2.18	0.64
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:O	1:A:315:THR:HG22	1.98	0.63
1:A:138:GLU:OE1	1:A:359:ILE:HD11	1.98	0.63
1:A:233:PHE:O	1:A:234:ASP:C	2.36	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:139:VAL:HG12	1:A:142:SER:HB3	1.81	0.62
1:A:66:ARG:HH11	1:A:66:ARG:CG	2.11	0.62
1:B:81:ASP:HA	1:B:84:LEU:HD12	1.82	0.61
1:A:305:GLN:HA	1:A:306:PRO:C	2.20	0.61
1:B:81:ASP:HA	1:B:84:LEU:CD1	2.30	0.60
1:B:305:GLN:HA	1:B:306:PRO:C	2.21	0.60
1:B:84:LEU:CD2	1:B:84:LEU:C	2.69	0.60
1:A:51:LEU:CD1	1:A:57:ILE:HD13	2.23	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:95:PHE:CE2	1:B:328:MET:HE2	2.39	0.58
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: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: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:A:217:TYR:CD1	1:A:217:TYR:C	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:VAL:HG13	1:B:357:ASP:O	2.06	0.55
1:A:164:GLU:OE2	1:A:167:ARG:HD3	2.06	0.55
1:A:38:LEU:HD12	1:A:73:LEU:O	2.05	0.55
1:A:167:ARG:HH22	1:A:173:GLU:CD	2.09	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:O	1:B:119:VAL:HG12	2.05	0.54
1:B:326:SER:H	1:B:328:MET:H	1.54	0.54
1:B:233:PHE:O	1:B:234:ASP:C	2.46	0.53
1:B:72:ILE:C	1:B:73:LEU:HD23	2.28	0.53
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: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:B:326:SER:C	1:B:328:MET:H	2.13	0.52
1:A:218:ASP:CG	2:A:401:NAD:HO2A	2.14	0.51
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: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:187:GLN:O	1:B:188:HIS:HB2	2.12	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: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:186:LEU:HD11	1:B:191:ILE:HD11	1.95	0.49
1:B:73:LEU:HD13	1:B:80:LEU:CB	2.42	0.49
1:A:62:PHE:O	1:A:66:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG2	1:A:315:THR:O	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:298:ALA:HB2	1:A:320:ALA:HB3	1.96	0.48
1:A:43:VAL:HB	1:A:46:GLN:HG3	1.94	0.48
1:B:362:SER:N	1:B:365:ILE:CG2	2.76	0.48
1:B:86:ASP:OD1	1:B:86:ASP:N	2.46	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
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:HA	1:B:164:GLU:OE1	2.15	0.47
1:B:168:GLN:HE21	1:B:178:GLN:HG2	1.80	0.47
1:B:362:SER:O	1:B:364:ARG:N	2.48	0.47
1:B:208:ALA:N	1:B:209:PRO:CD	2.78	0.47
1:B:302:TRP:HB2	1:B:305:GLN:HG3	1.97	0.47
1:B:66:ARG:HH11	1:B:66:ARG:HG3	1.79	0.47
1:A:291:SER:C	1:A:292:GLU:HG3	2.34	0.46
1:A:250:THR:HB	1:A:251:PRO:CD	2.46	0.46
1:B:48:ASN:OD1	1:B:48:ASN:C	2.53	0.46
1:A:205:GLU:HA	1:A:227:LEU:HD21	1.97	0.46
1:B:102:ARG:NH1	1:B:102:ARG:CB	2.51	0.46
1:B:89:VAL:HG22	1:B:113:LEU:HB3	1.97	0.46
1:A:311:HIS:ND1	1:A:312:PRO:HD2	2.31	0.46
1:A:159:LEU:HD13	1:A:186:LEU:CD1	2.45	0.46
1:B:326:SER:C	1:B:328:MET:N	2.70	0.46
1:A:243:ILE:HD12	1:A:265:MET:CE	2.46	0.45
1:A:303:TYR:HA	1:A:304:PRO:HA	1.79	0.45
1:B:84:LEU:HD22	1:B:84:LEU:C	2.35	0.45
1:B:95:PHE:CE2	1:B:328:MET:HE1	2.50	0.45
1:A:190:THR:C	1:A:191:ILE:HD13	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:115:ILE:CD1	1:A:344:LEU:HD21	2.48	0.44
1:A:48:ASN:HB2	1:B:181:ASN:CG	2.38	0.44
1:A:60:LYS:HE2	1:A:60:LYS:HB2	1.21	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:HA	1:A:330:LEU:HD12	1.75	0.44
1:A:343:ILE:HG22	1:A:344:LEU:N	2.33	0.44
1:A:86:ASP:OD1	1:A:86:ASP:N	2.51	0.44
1:A:225:HIS:CE1	1:A:227:LEU:HB2	2.52	0.44
1:A:328:MET:HG2	1:A:328:MET:O	2.18	0.44
1:A:159:LEU:CD1	1:A:186:LEU:HD13	2.47	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
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:175:ASN:CB	1:B:178:GLN:HB3	2.49	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:CG	1:B:102:ARG:HH11	2.27	0.43
1:B:231:VAL:HG13	1:B:232:SER:O	2.19	0.43
1:B:84:LEU:HD23	1:B:84:LEU:C	2.38	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:135:GLY:HA3	1:B:365:ILE:HD13	2.01	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:A:237:VAL:O	1:A:265:MET:HA	2.19	0.42
1:A:49:GLN:HB3	1:A:52:ASN:ND2	2.34	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:A:167:ARG:NH2	1:A:173:GLU:CD	2.73	0.42
1:B:330:LEU:HA	1:B:330:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LYS:HG3	1:B:259:LYS:O	2.19	0.42
1:B:275:ALA:C	1:B:276:ARG:HG2	2.40	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:261:VAL:O	1:A:262:LEU:C	2.55	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:158:LEU:HD21	1:A:298:ALA:N	2.35	0.41
1:A:60:LYS:HA	1:A:70:PHE:CD2	2.55	0.41
1:A:168:GLN:HA	1:A:173:GLU:HB2	2.03	0.41
1:A:89:VAL:HG22	1:A:113:LEU:HB3	2.02	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:B:56:ALA:C	1:B:57:ILE:HG12	2.40	0.41
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.84	0.41
1:A:275:ALA:C	1:A:276:ARG:HG2	2.40	0.41
1:B:289:LEU:O	1:B:292:GLU:N	2.50	0.41
1:A:208:ALA:HB3	1:A:209:PRO:HD3	2.01	0.41
1:A:52:ASN:O	1:A:56:ALA:HA	2.20	0.41
1:B:262:LEU:HD12	1:B:262:LEU:HA	1.82	0.41
1:A:184:HIS:HA	1:B:331:GLU:OE1	2.21	0.41
1:A:84:LEU:HD21	1:A:104:ARG:CG	2.45	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:B:344:LEU:O	1:B:348:PHE:CD2	2.73	0.41
1:B:97:PRO:HB3	1:B:123:HIS:CG	2.56	0.41
1:A:43:VAL:HG23	1:B:177:SER:HB2	2.03	0.40
1:B:235:GLU:O	1:B:236:LEU:C	2.58	0.40
1:B:282:ARG:NH2	1:B:303:TYR:O	2.54	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:225:HIS:ND1	1:A:227:LEU:N	2.70	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	329/373 (88%)	291 (88%)	33 (10%)	5 (2%)	10 26
1	B	321/373 (86%)	282 (88%)	31 (10%)	8 (2%)	5 14
All	All	650/746 (87%)	573 (88%)	64 (10%)	13 (2%)	7 19

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%)	232 (89%)	28 (11%)	6 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	252/317 (80%)	220 (87%)	32 (13%)	4 10
All	All	512/634 (81%)	452 (88%)	60 (12%)	5 12

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

Mol	Chain	Res	Type
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	107	LYS
1	A	122	ASP
1	A	155	LEU
1	A	158	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	252	GLU
1	A	264	ARG
1	A	266	LYS
1	A	276	ARG
1	A	289	LEU
1	A	294	LEU
1	A	304	PRO
1	A	330	LEU
1	B	38	LEU
1	B	52	ASN
1	B	59	LEU
1	B	61	THR
1	B	65	GLU
1	B	69	GLU
1	B	83	HIS
1	B	84	LEU

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Mol	Chain	Res	Type
1	B	102	ARG
1	B	119	VAL
1	B	140	THR
1	B	159	LEU
1	B	171	GLU
1	B	175	ASN
1	B	191	ILE
1	B	198	ARG
1	B	202	LEU
1	B	221	ASN
1	B	231	VAL
1	B	250	THR
1	B	252	GLU
1	B	260	ASP
1	B	262	LEU
1	B	266	LYS
1	B	276	ARG
1	B	289	LEU
1	B	315	THR
1	B	328	MET
1	B	330	LEU
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	110	ASN
1	A	133	ASN
1	A	178	GLN
1	A	188	HIS
1	A	211	ASN
1	B	187	GLN
1	B	211	ASN
1	B	255	ASN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

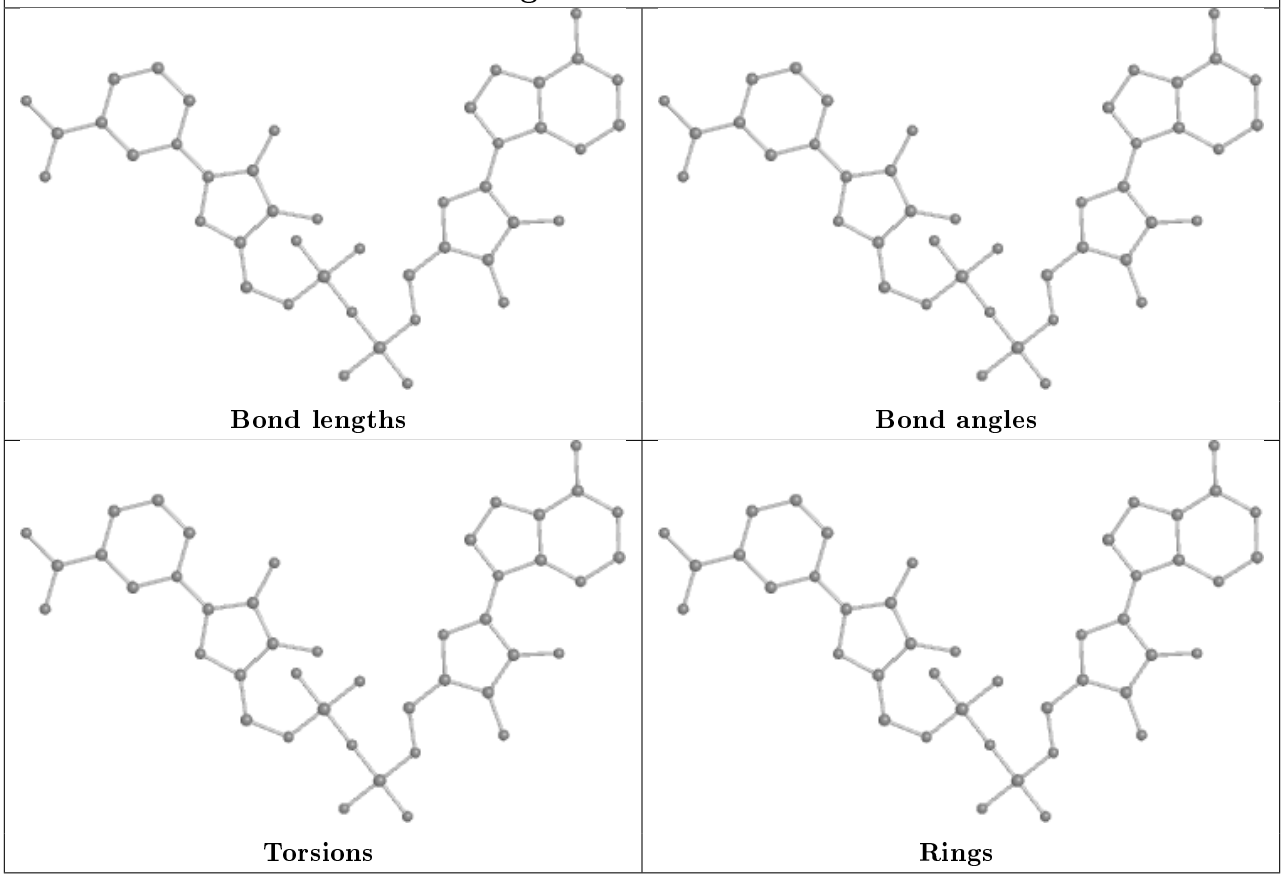
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

Ligand NAD A 401



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

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, 95^{th} 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%)	-0.25	0 100 100	10, 24, 41, 76	0
1	B	327/373 (87%)	-0.05	2 (0%) 89 91	12, 28, 53, 101	0
All	All	658/746 (88%)	-0.15	2 (0%) 94 95	10, 26, 50, 101	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	141	GLY	2.9
1	B	85	PRO	2.5

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 monosaccharides 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, 95^{th} 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.

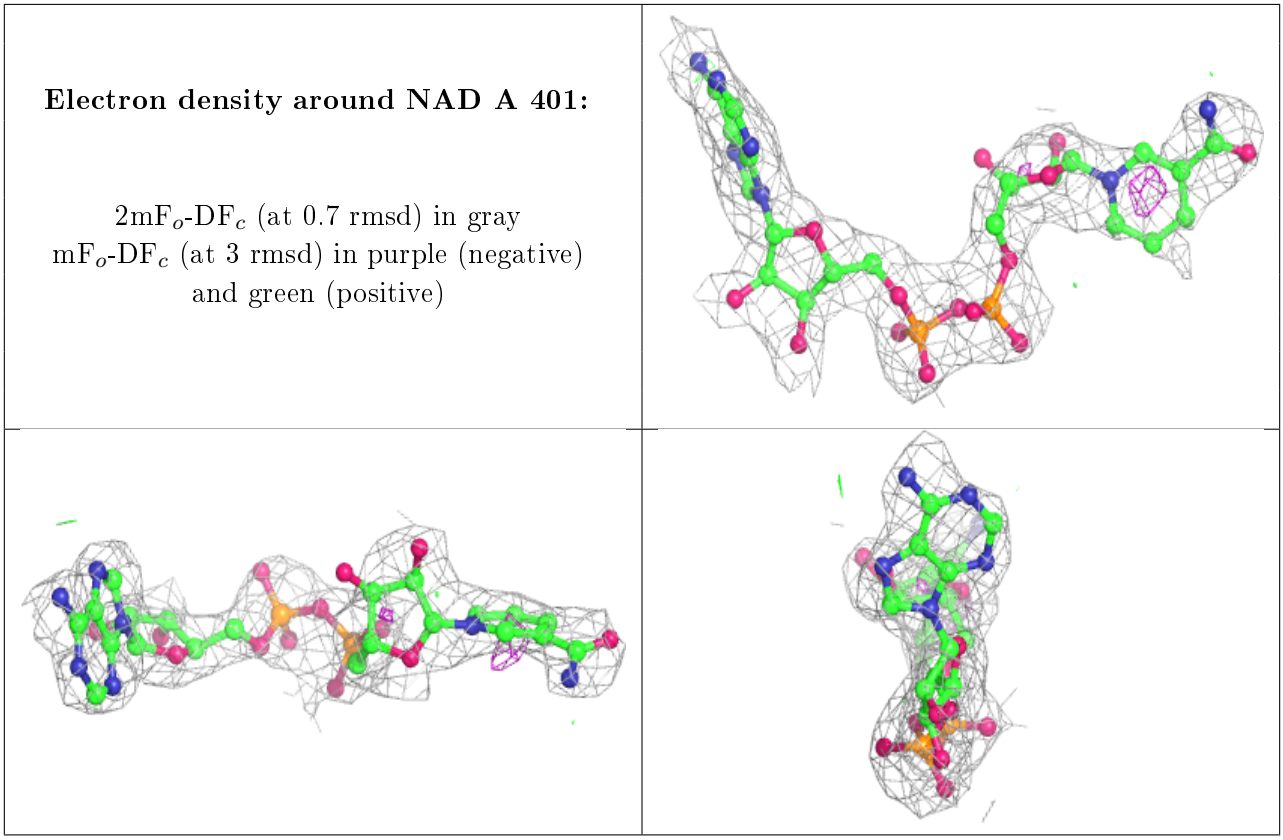
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	A	401	44/44	0.94	0.23	33,47,58,70	0

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.

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)



6.5 Other polymers

There are no such residues in this entry.