



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:10 AM UTC

PDB ID : 1MFP / pdb_00001mfp
Title : E. coli Enoyl Reductase in complex with NAD and SB611113
Authors : Seefeld, M.A.; Miller, W.H.; Newlander, K.A.; Burgess, W.J.; DeWolf Jr., W.E.; Elkins, P.A.; Head, M.S.; Jakas, D.R.; Janson, C.A.; Keller, P.M.; Manley, P.J.; Moore, T.D.; Payne, D.J.; Pearson, S.; Polizzi, B.J.; Qiu, X.; Rittenhouse, S.F.; Uzinskas, I.N.; Wallis, N.G.; Huffman, W.F.
Deposited on : 2002-08-13
Resolution : 2.33 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (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

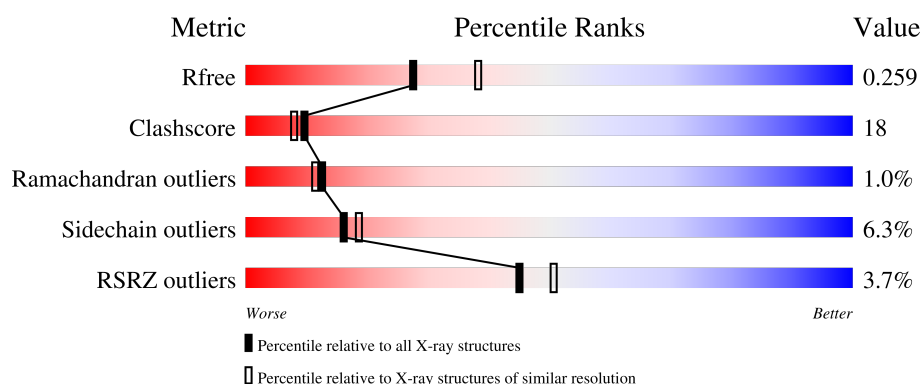
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	262	4% 58% 34% 6%
1	B	262	3% 63% 30% 6%

2 Entry composition [i](#)

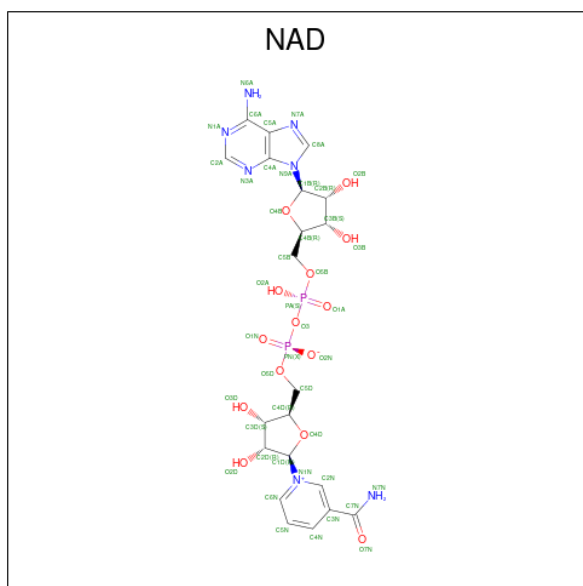
There are 5 unique types of molecules in this entry. The entry contains 4180 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 enoyl-[acyl-carrier-protein] reductase [Nadh].

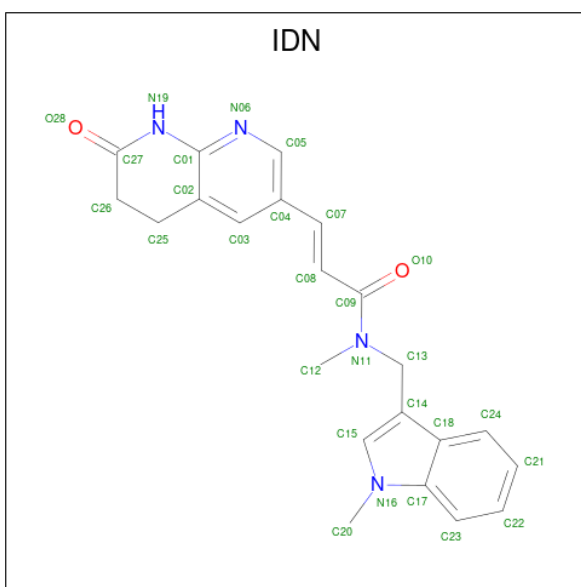
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1918	1209	331	365	13			
1	B	258	Total	C	N	O	S	0	0	0
			1918	1209	331	365	13			

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



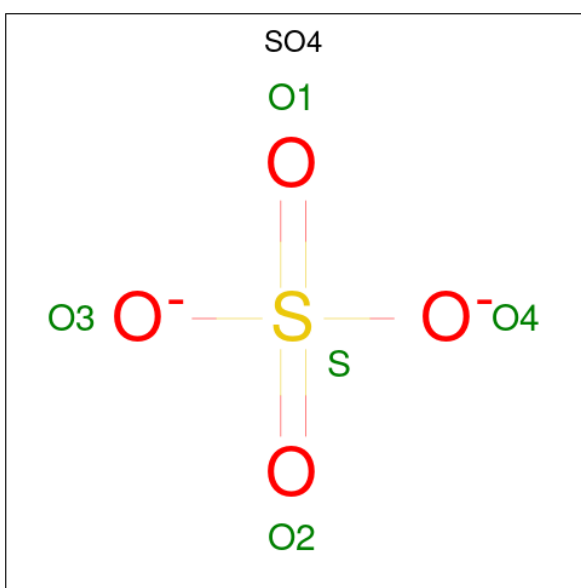
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is (E)-N-METHYL-N-(1-METHYL-1H-INDOL-3-YLMETHYL)-3-(7-OXO-5,6,7,8-TETRAHYDRO-[1,8]NAPHTHYRIDIN-3-YL)-ACRYLAMIDE (CCD ID: IDN) (formula: $C_{22}H_{22}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	22	4	2		
3	B	1	Total	C	N	O	0	0
			28	22	4	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

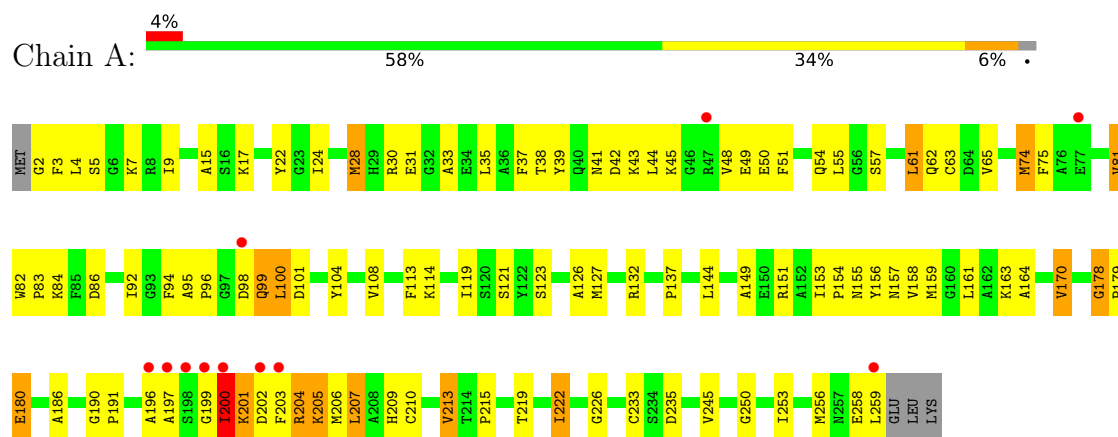
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	86	Total 86	O 86	0	0
5	B	109	Total 109	O 109	0	0

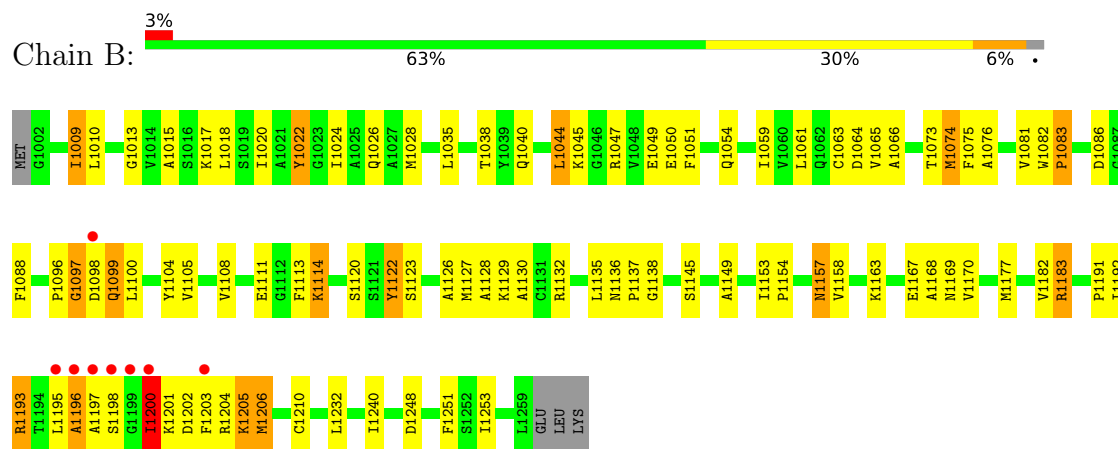
3 Residue-property plots [i](#)

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: enoyl-[acyl-carrier-protein] reductase [Nadh]



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4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.60Å 79.60Å 325.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.33 20.00 – 2.33	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.33) 69.1 (20.00-2.33)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.86 (at 2.33Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.259 0.198 , 0.259	Depositor DCC
R_{free} test set	933 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4180	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: SO4, NAD, IDN

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	1.11	5/1950 (0.3%)	1.32	23/2634 (0.9%)
1	B	1.13	3/1950 (0.2%)	1.34	20/2634 (0.8%)
All	All	1.12	8/3900 (0.2%)	1.33	43/5268 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1074	MET	SD-CE	10.12	2.04	1.79
1	A	74	MET	SD-CE	6.93	1.96	1.79
1	A	28	MET	SD-CE	6.34	1.95	1.79
1	B	1127	MET	SD-CE	6.04	1.94	1.79
1	A	245	VAL	CA-CB	5.67	1.61	1.54
1	B	1105	VAL	CA-CB	5.42	1.61	1.54
1	A	127	MET	SD-CE	5.16	1.92	1.79
1	A	213	VAL	CA-CB	5.01	1.60	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1099	GLN	N-CA-C	8.54	121.53	111.71
1	B	1086	ASP	N-CA-C	7.45	121.68	112.59
1	A	9	ILE	N-CA-C	7.39	118.54	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1136	ASN	CA-C-N	-7.23	112.55	119.85
1	B	1136	ASN	C-N-CA	-7.23	112.55	119.85
1	A	100	LEU	N-CA-C	7.00	121.13	111.55
1	B	1013	GLY	N-CA-C	6.98	124.95	115.32
1	A	199	GLY	N-CA-C	6.75	125.02	115.30
1	A	156	TYR	N-CA-C	-6.71	104.00	111.71
1	B	1020	ILE	N-CA-C	-6.69	104.24	110.53
1	A	99	GLN	N-CA-C	6.50	119.18	111.71
1	B	1083	PRO	N-CA-C	-6.50	104.39	113.81
1	A	57	SER	N-CA-C	6.44	119.89	109.40
1	A	121	SER	N-CA-C	6.13	120.56	112.72
1	A	200	ILE	N-CA-C	6.07	120.91	112.35
1	A	126	ALA	N-CA-C	-6.04	104.61	111.07
1	A	61	LEU	N-CA-C	5.96	119.12	109.40
1	A	119	ILE	CB-CA-C	-5.90	104.33	112.24
1	B	1177	MET	N-CA-C	5.88	120.46	113.28
1	B	1035	LEU	N-CA-C	5.86	119.61	110.17
1	B	1132	ARG	N-CA-C	5.85	118.13	111.11
1	A	132	ARG	N-CA-C	5.79	118.06	111.11
1	A	222	ILE	N-CA-C	-5.75	105.52	113.00
1	B	1009	ILE	N-CA-C	5.75	116.15	108.11
1	B	1138	GLY	N-CA-C	-5.72	107.48	114.92
1	A	86	ASP	N-CA-C	5.71	120.25	112.88
1	B	1076	ALA	N-CA-C	-5.69	105.00	111.14
1	B	1183	ARG	N-CA-C	-5.67	101.64	110.42
1	A	35	LEU	N-CA-C	5.66	119.19	110.42
1	B	1130	ALA	N-CA-C	5.64	118.20	111.71
1	A	178	GLY	CA-C-N	5.52	125.19	119.56
1	A	178	GLY	C-N-CA	5.52	125.19	119.56
1	A	137	PRO	N-CA-C	-5.50	102.63	111.38
1	B	1168	ALA	N-CA-C	-5.46	105.40	111.36
1	B	1135	LEU	N-CA-C	5.43	118.48	109.46
1	B	1137	PRO	N-CA-C	-5.43	102.75	111.38
1	B	1200	ILE	N-CA-C	5.43	115.93	108.12
1	A	164	ALA	N-CA-C	-5.34	105.54	111.36
1	B	1114	LYS	N-CA-C	5.33	117.50	111.11
1	A	190	GLY	N-CA-C	-5.29	105.59	112.10
1	A	170	VAL	CB-CA-C	-5.27	105.13	111.88
1	A	219	THR	N-CA-C	-5.14	102.91	110.52
1	A	92	ILE	N-CA-C	5.07	115.28	107.77

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1022	TYR	Sidechain
1	B	1122	TYR	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	1918	0	1909	76	0
1	B	1918	0	1909	67	0
2	A	44	0	26	2	0
2	B	44	0	26	3	0
3	A	28	0	22	4	0
3	B	28	0	22	4	0
4	B	5	0	0	0	0
5	A	86	0	0	4	0
5	B	109	0	0	3	0
All	All	4180	0	3914	140	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 18.

All (140) 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:B:1074:MET:SD	1:B:1074:MET:CE	2.04	1.45
1:B:1191:PRO:HG3	1:B:1206:MET:HE1	1.45	0.95
1:B:1099:GLN:HE22	1:B:1108:VAL:HA	1.42	0.84
1:A:202:ASP:OD2	1:A:204:ARG:HG2	1.82	0.80
1:B:1038:THR:HA	1:B:1061:LEU:O	1.83	0.79
1:A:99:GLN:HE22	1:A:108:VAL:HA	1.54	0.73
1:A:256:MET:HB3	1:A:259:LEU:HD13	1.71	0.71
1:A:197:ALA:HB1	1:A:203:PHE:CE2	2.27	0.70
1:A:17:LYS:HA	1:A:22:TYR:CD1	2.27	0.69
1:A:259:LEU:H	1:A:259:LEU:HD12	1.56	0.69
1:B:1191:PRO:HG3	1:B:1206:MET:CE	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1192:ILE:HA	5:B:138:HOH:O	1.95	0.66
1:B:1024:ILE:O	1:B:1028:MET:HG3	1.95	0.65
1:A:196:ALA:O	3:A:302:IDN:H251	1.96	0.64
1:B:1191:PRO:CG	1:B:1206:MET:HE1	2.24	0.64
1:A:155:ASN:HD22	1:A:201:LYS:HD3	1.63	0.64
1:B:1099:GLN:NE2	1:B:1108:VAL:HA	2.13	0.62
1:A:256:MET:HE2	1:A:259:LEU:HD21	1.82	0.62
1:B:1050:GLU:OE2	1:B:1054:GLN:NE2	2.33	0.62
1:A:108:VAL:O	1:B:1129:LYS:CE	2.48	0.61
1:A:202:ASP:OD2	1:A:204:ARG:CG	2.48	0.61
1:A:180:GLU:OE1	5:A:382:HOH:O	2.16	0.61
1:A:205:LYS:HE2	1:A:205:LYS:HA	1.81	0.61
1:A:209:HIS:O	1:A:213:VAL:HG22	2.01	0.61
1:A:114:LYS:HD2	1:A:114:LYS:C	2.26	0.61
1:A:200:ILE:HB	3:A:302:IDN:H202	1.83	0.61
1:B:1017:LYS:HE2	1:B:1022:TYR:OH	2.02	0.59
1:B:1197:ALA:O	1:B:1200:ILE:HG12	2.02	0.59
1:B:1200:ILE:HD11	3:B:1302:IDN:H15	1.85	0.59
1:A:38:THR:HA	1:A:61:LEU:O	2.03	0.58
1:A:81:VAL:O	1:A:82:TRP:HD1	1.86	0.58
1:B:1205:LYS:NZ	1:B:1205:LYS:HA	2.19	0.58
1:B:1047:ARG:NH1	1:B:1051:PHE:CZ	2.72	0.58
1:B:1047:ARG:HA	1:B:1047:ARG:HE	1.68	0.57
1:A:108:VAL:O	1:B:1129:LYS:HE2	2.04	0.56
1:A:222:ILE:HG23	5:A:365:HOH:O	2.06	0.56
1:A:81:VAL:HG22	1:A:82:TRP:CD1	2.42	0.55
1:B:1045:LYS:O	1:B:1049:GLU:HG3	2.06	0.55
1:B:1253:ILE:C	1:B:1253:ILE:HD12	2.31	0.55
1:A:104:TYR:HD1	1:A:157:ASN:HB3	1.71	0.54
1:A:65:VAL:HG22	2:A:301:NAD:N1A	2.22	0.54
1:B:1099:GLN:C	1:B:1100:LEU:HD23	2.32	0.54
1:B:1047:ARG:CZ	1:B:1051:PHE:CZ	2.91	0.54
1:B:1064:ASP:OD1	1:B:1066:ALA:HB3	2.08	0.53
1:B:1182:VAL:HG12	1:B:1183:ARG:O	2.09	0.53
1:B:1206:MET:HE2	1:B:1210:CYS:SG	2.49	0.53
1:A:250:GLY:O	1:A:253:ILE:HG13	2.09	0.53
1:B:1104:TYR:HD1	1:B:1157:ASN:HB3	1.74	0.53
1:B:1044:LEU:HD23	5:B:181:HOH:O	2.08	0.52
1:B:1193:ARG:O	1:B:1193:ARG:HG3	2.09	0.52
1:B:1063:CYS:HB2	1:B:1074:MET:HG3	1.92	0.52
1:A:50:GLU:O	1:A:54:GLN:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1010:LEU:HB3	1:B:1088:PHE:HB3	1.92	0.51
1:B:1065:VAL:HB	1:B:1123:SER:HB2	1.93	0.51
1:A:201:LYS:HG3	1:A:202:ASP:N	2.26	0.50
1:B:1017:LYS:HG2	1:B:1022:TYR:CZ	2.46	0.50
1:A:204:ARG:HG2	1:A:205:LYS:H	1.76	0.50
1:B:1010:LEU:HD11	1:B:1038:THR:HG23	1.92	0.50
1:A:149:ALA:HB2	1:A:163:LYS:HB3	1.93	0.50
1:B:1047:ARG:HE	1:B:1047:ARG:CA	2.25	0.50
1:A:24:ILE:HG12	1:A:226:GLY:HA2	1.93	0.49
2:B:1301:NAD:C4N	3:B:1302:IDN:H122	2.43	0.49
1:A:178:GLY:N	1:A:179:PRO:CD	2.75	0.49
1:A:170:VAL:HG21	1:A:186:ALA:HB2	1.93	0.49
1:B:1196:ALA:O	3:B:1302:IDN:H03	2.12	0.49
1:B:1074:MET:HE1	1:B:1075:PHE:CZ	2.47	0.49
1:B:1201:LYS:HG3	1:B:1202:ASP:N	2.28	0.49
1:A:28:MET:HE2	1:A:233:CYS:HB2	1.94	0.49
1:B:1015:ALA:HB2	2:B:1301:NAD:O3B	2.13	0.49
1:A:74:MET:HE1	1:A:75:PHE:CZ	2.48	0.48
1:B:1022:TYR:OH	1:B:1026:GLN:NE2	2.46	0.48
1:B:1114:LYS:C	1:B:1114:LYS:HD3	2.38	0.48
1:A:258:GLU:HG2	1:A:259:LEU:HD12	1.95	0.48
1:B:1183:ARG:HD2	1:B:1240:ILE:O	2.13	0.48
1:B:1248:ASP:OD2	1:B:1251:PHE:HB3	2.14	0.48
1:A:3:PHE:CZ	1:A:31:GLU:HG3	2.49	0.48
1:A:37:PHE:CD1	1:A:37:PHE:N	2.81	0.48
1:B:1167:GLU:O	1:B:1170:VAL:HB	2.13	0.48
1:A:206:MET:HE3	1:A:206:MET:HB3	1.75	0.48
1:A:155:ASN:HD22	1:A:201:LYS:CD	2.26	0.47
1:A:99:GLN:NE2	1:A:108:VAL:HA	2.26	0.47
1:B:1128:ALA:O	1:B:1129:LYS:C	2.53	0.46
1:A:159:MET:CE	1:A:163:LYS:HE2	2.45	0.46
1:A:30:ARG:NE	1:A:31:GLU:OE2	2.46	0.46
1:A:191:PRO:HG2	1:A:210:CYS:SG	2.56	0.46
1:A:62:GLN:NE2	1:A:63:CYS:N	2.64	0.45
1:B:1009:ILE:HD13	1:B:1028:MET:CE	2.47	0.45
1:A:258:GLU:O	1:A:259:LEU:C	2.60	0.45
1:A:44:LEU:O	1:A:48:VAL:HG23	2.16	0.45
1:A:197:ALA:O	1:A:200:ILE:HD11	2.17	0.45
1:A:4:LEU:HB3	1:A:33:ALA:HB2	1.99	0.45
1:A:7:LYS:NZ	5:A:312:HOH:O	2.32	0.45
1:B:1096:PRO:O	1:B:1097:GLY:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:HG22	1:A:158:VAL:O	2.17	0.44
1:B:1017:LYS:HG2	1:B:1022:TYR:CE2	2.52	0.44
1:A:42:ASP:O	1:A:43:LYS:C	2.58	0.44
1:B:1047:ARG:HA	1:B:1047:ARG:NE	2.31	0.44
1:A:65:VAL:HB	1:A:123:SER:HB2	2.00	0.44
1:A:113:PHE:CD1	1:A:113:PHE:C	2.95	0.44
1:B:1200:ILE:CD1	3:B:1302:IDN:H15	2.48	0.44
1:A:48:VAL:HA	1:A:51:PHE:CD1	2.52	0.44
1:B:1145:SER:HA	1:B:1163:LYS:HD2	2.00	0.43
1:B:1059:ILE:HD11	1:B:1081:VAL:HG11	1.99	0.43
1:A:55:LEU:HD23	1:A:55:LEU:HA	1.68	0.43
1:A:108:VAL:O	1:B:1129:LYS:HE3	2.17	0.43
1:B:1196:ALA:HB2	2:B:1301:NAD:O1A	2.18	0.43
1:B:1082:TRP:O	1:B:1083:PRO:C	2.62	0.42
1:B:1122:TYR:CE2	1:B:1126:ALA:HB2	2.54	0.42
1:A:200:ILE:CB	3:A:302:IDN:H202	2.49	0.42
1:A:94:PHE:HA	3:A:302:IDN:N06	2.34	0.42
1:A:2:GLY:N	1:A:5:SER:HG	2.17	0.42
1:B:1232:LEU:HD23	1:B:1232:LEU:HA	1.82	0.42
1:B:1059:ILE:CD1	1:B:1081:VAL:HG11	2.49	0.42
1:B:1047:ARG:HH21	1:B:1050:GLU:HB3	1.85	0.42
1:A:82:TRP:O	1:A:83:PRO:C	2.62	0.42
1:A:94:PHE:CG	1:A:95:ALA:N	2.88	0.42
1:A:153:ILE:HA	1:A:154:PRO:HD3	1.95	0.42
1:A:235:ASP:OD2	5:A:345:HOH:O	2.21	0.42
1:A:161:LEU:HD21	1:B:1169:ASN:CG	2.45	0.42
1:A:15:ALA:HB2	2:A:301:NAD:O3B	2.20	0.41
1:B:1205:LYS:HA	1:B:1205:LYS:HZ3	1.84	0.41
1:A:259:LEU:H	1:A:259:LEU:CD1	2.29	0.41
1:A:39:TYR:HD2	1:A:41:ASN:O	2.02	0.41
1:A:253:ILE:C	1:A:253:ILE:HD12	2.45	0.41
1:B:1153:ILE:O	1:B:1154:PRO:C	2.62	0.41
1:A:205:LYS:HA	1:A:205:LYS:CE	2.49	0.41
1:B:1253:ILE:C	1:B:1253:ILE:CD1	2.94	0.41
1:A:30:ARG:NH2	1:A:31:GLU:OE2	2.50	0.41
1:A:95:ALA:O	1:A:96:PRO:C	2.62	0.41
1:A:203:PHE:O	1:A:206:MET:HB3	2.21	0.41
1:B:1098:ASP:OD1	1:B:1098:ASP:N	2.53	0.41
1:B:1149:ALA:HB2	1:B:1163:LYS:HB3	2.02	0.41
1:A:44:LEU:N	1:A:44:LEU:HD12	2.36	0.41
1:A:45:LYS:O	1:A:49:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD12	1:A:207:LEU:HA	1.78	0.41
1:B:1197:ALA:HB1	1:B:1203:PHE:CE2	2.56	0.41
1:A:256:MET:CB	1:A:259:LEU:HD13	2.46	0.40
1:A:259:LEU:HD12	1:A:259:LEU:N	2.32	0.40
1:B:1040:GLN:NE2	5:B:165:HOH:O	2.55	0.40
1:B:1113:PHE:CD1	1:B:1113:PHE:C	2.99	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	256/262 (98%)	240 (94%)	15 (6%)	1 (0%)	30	32
1	B	256/262 (98%)	236 (92%)	16 (6%)	4 (2%)	7	5
All	All	512/524 (98%)	476 (93%)	31 (6%)	5 (1%)	12	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1196	ALA
1	B	1198	SER
1	A	201	LYS
1	B	1157	ASN
1	B	1097	GLY

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	197/201 (98%)	184 (93%)	13 (7%)	15	17
1	B	197/201 (98%)	185 (94%)	12 (6%)	17	20
All	All	394/402 (98%)	369 (94%)	25 (6%)	16	19

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	VAL
1	A	84	LYS
1	A	98	ASP
1	A	100	LEU
1	A	101	ASP
1	A	144	LEU
1	A	151	ARG
1	A	180	GLU
1	A	200	ILE
1	A	204	ARG
1	A	205	LYS
1	A	207	LEU
1	A	215	PRO
1	B	1018	LEU
1	B	1044	LEU
1	B	1073	THR
1	B	1111	GLU
1	B	1120	SER
1	B	1158	VAL
1	B	1193	ARG
1	B	1195	LEU
1	B	1200	ILE
1	B	1204	ARG
1	B	1205	LYS
1	B	1206	MET

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	26	GLN
1	A	40	GLN

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Mol	Chain	Res	Type
1	A	62	GLN
1	A	99	GLN
1	A	155	ASN
1	A	169	ASN
1	A	175	ASN
1	A	257	ASN
1	B	1026	GLN
1	B	1062	GLN
1	B	1099	GLN
1	B	1169	ASN
1	B	1257	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](#)

5 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	$\# Z > 2$
3	IDN	A	302	-	31,31,31	3.10	20 (64%)	39,44,44	1.62	4 (10%)
2	NAD	A	301	-	46,48,48	2.08	11 (23%)	64,73,73	1.86	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IDN	B	1302	-	31,31,31	2.87	18 (58%)	39,44,44	1.76	4 (10%)
4	SO4	B	1303	-	4,4,4	0.48	0	6,6,6	0.20	0
2	NAD	B	1301	-	46,48,48	2.18	10 (21%)	64,73,73	1.85	14 (21%)

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	301	-	-	8/30/62/62	0/5/5/5
3	IDN	A	302	-	-	4/13/22/22	0/4/4/4
2	NAD	B	1301	-	-	10/30/62/62	0/5/5/5
3	IDN	B	1302	-	-	4/13/22/22	0/4/4/4

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAD	C2N-N1N	8.07	1.43	1.35
2	B	1301	NAD	C2N-N1N	7.23	1.42	1.35
3	B	1302	IDN	C02-C01	6.43	1.47	1.41
3	A	302	IDN	C02-C01	6.25	1.47	1.41
2	B	1301	NAD	PA-O3	6.06	1.66	1.59
3	A	302	IDN	C09-N11	6.03	1.43	1.35
3	B	1302	IDN	C18-C17	5.63	1.48	1.41
3	B	1302	IDN	C09-N11	5.24	1.42	1.35
2	B	1301	NAD	O4D-C1D	5.19	1.47	1.40
3	A	302	IDN	C18-C17	5.04	1.47	1.41
2	A	301	NAD	O4D-C1D	4.71	1.47	1.40
2	A	301	NAD	C5A-N7A	-4.37	1.31	1.39
3	A	302	IDN	C05-C04	4.33	1.46	1.39
3	A	302	IDN	C27-N19	4.26	1.40	1.35
2	B	1301	NAD	C5A-N7A	-4.13	1.31	1.39
3	A	302	IDN	C22-C23	4.04	1.45	1.38
3	B	1302	IDN	C22-C23	4.03	1.45	1.38
3	A	302	IDN	C21-C24	3.95	1.45	1.38
2	B	1301	NAD	C2N-C3N	3.85	1.45	1.39
3	B	1302	IDN	C26-C27	3.70	1.58	1.50
3	B	1302	IDN	C03-C02	3.63	1.45	1.39
3	A	302	IDN	C26-C27	3.60	1.57	1.50
3	A	302	IDN	C03-C02	3.57	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1302	IDN	C17-N16	3.42	1.43	1.38
3	A	302	IDN	C23-C17	3.37	1.44	1.39
3	A	302	IDN	C05-N06	3.35	1.41	1.34
3	B	1302	IDN	C05-C04	3.35	1.44	1.39
2	A	301	NAD	C3N-C7N	3.21	1.55	1.50
3	B	1302	IDN	C21-C24	3.19	1.44	1.38
3	B	1302	IDN	C22-C21	3.17	1.45	1.38
3	A	302	IDN	C22-C21	3.16	1.45	1.38
2	A	301	NAD	C6N-N1N	3.16	1.42	1.35
3	A	302	IDN	C17-N16	3.13	1.42	1.38
2	B	1301	NAD	C4N-C3N	2.99	1.43	1.39
2	A	301	NAD	C5N-C4N	2.98	1.44	1.38
2	B	1301	NAD	PN-O3	2.89	1.62	1.59
3	A	302	IDN	C01-N06	2.89	1.39	1.35
3	B	1302	IDN	C03-C04	2.88	1.44	1.39
3	B	1302	IDN	C23-C17	2.86	1.44	1.39
3	B	1302	IDN	C27-N19	2.80	1.38	1.35
2	A	301	NAD	C4A-N9A	-2.79	1.31	1.37
2	A	301	NAD	C4N-C3N	2.79	1.43	1.39
3	A	302	IDN	C08-C09	2.79	1.52	1.48
2	A	301	NAD	C2A-N1A	2.79	1.38	1.33
3	A	302	IDN	C03-C04	2.72	1.44	1.39
3	A	302	IDN	C24-C18	2.72	1.44	1.39
3	B	1302	IDN	C05-N06	2.71	1.39	1.34
2	B	1301	NAD	C6N-N1N	2.65	1.41	1.35
3	A	302	IDN	C08-C07	2.61	1.39	1.33
2	A	301	NAD	C4A-N3A	2.57	1.39	1.34
3	B	1302	IDN	C15-C14	2.56	1.42	1.36
2	B	1301	NAD	C4A-N9A	-2.45	1.32	1.37
3	B	1302	IDN	C20-N16	2.44	1.50	1.46
3	A	302	IDN	C25-C26	2.36	1.57	1.52
3	B	1302	IDN	C25-C26	2.33	1.57	1.52
2	B	1301	NAD	C3N-C7N	2.32	1.54	1.50
3	A	302	IDN	C15-C14	2.23	1.41	1.36
3	B	1302	IDN	C01-N06	2.11	1.38	1.35
2	A	301	NAD	C2A-N3A	2.07	1.37	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1302	IDN	C08-C09-N11	7.23	122.78	117.91
3	A	302	IDN	C08-C09-N11	6.33	122.17	117.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	NAD	C4B-O4B-C1B	-5.58	97.15	109.47
2	B	1301	NAD	N3A-C4A-N9A	5.50	136.52	127.17
2	A	301	NAD	N3A-C4A-N9A	5.48	136.49	127.17
2	A	301	NAD	C4B-O4B-C1B	-5.17	98.05	109.47
2	A	301	NAD	N3A-C2A-N1A	-4.99	121.03	128.58
2	B	1301	NAD	C5A-C4A-N3A	-4.97	119.87	126.72
2	B	1301	NAD	N3A-C2A-N1A	-4.39	121.94	128.58
2	A	301	NAD	C5A-C4A-N3A	-4.25	120.87	126.72
3	B	1302	IDN	O10-C09-C08	-4.24	113.46	122.02
3	A	302	IDN	O10-C09-C08	-4.06	113.82	122.02
2	A	301	NAD	C4A-N9A-C8A	3.77	109.70	105.74
2	A	301	NAD	C6A-C5A-N7A	-3.56	125.22	132.09
2	B	1301	NAD	O4B-C1B-N9A	3.43	114.67	108.09
3	B	1302	IDN	C23-C17-N16	3.35	134.47	129.91
2	B	1301	NAD	C6A-C5A-N7A	-3.31	125.71	132.09
2	A	301	NAD	C6A-C5A-C4A	3.17	121.51	117.18
3	A	302	IDN	C23-C17-N16	3.07	134.10	129.91
3	B	1302	IDN	C23-C17-C18	-3.00	118.60	121.95
2	B	1301	NAD	C2A-N3A-C4A	2.94	119.01	111.83
2	A	301	NAD	C5A-C4A-N9A	-2.91	102.64	105.81
2	A	301	NAD	C2A-N3A-C4A	2.82	118.72	111.83
3	A	302	IDN	C23-C17-C18	-2.67	118.97	121.95
2	B	1301	NAD	C6A-C5A-C4A	2.61	120.74	117.18
2	B	1301	NAD	C4A-C5A-N7A	2.60	113.55	110.58
2	A	301	NAD	N6A-C6A-N1A	2.46	123.86	118.38
2	A	301	NAD	N9A-C8A-N7A	-2.40	110.53	113.94
2	B	1301	NAD	C4A-N9A-C1B	-2.37	121.10	126.63
2	B	1301	NAD	C4A-N9A-C8A	2.35	108.21	105.74
2	A	301	NAD	C4A-C5A-N7A	2.35	113.27	110.58
2	A	301	NAD	C4A-N9A-C1B	-2.23	121.43	126.63
2	A	301	NAD	O4B-C1B-N9A	2.07	112.07	108.09
2	B	1301	NAD	C4D-O4D-C1D	2.06	111.81	109.92
2	B	1301	NAD	C5A-C4A-N9A	-2.02	103.61	105.81
2	B	1301	NAD	N6A-C6A-N1A	2.01	122.86	118.38

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAD	PN-O3-PA-O5B
2	A	301	NAD	C5D-O5D-PN-O3
2	A	301	NAD	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	A	301	NAD	C5D-O5D-PN-O2N
2	A	301	NAD	O4D-C1D-N1N-C2N
2	A	301	NAD	O4D-C1D-N1N-C6N
2	B	1301	NAD	C5D-O5D-PN-O3
2	B	1301	NAD	C5D-O5D-PN-O1N
2	B	1301	NAD	C5D-O5D-PN-O2N
2	B	1301	NAD	O4D-C1D-N1N-C2N
3	A	302	IDN	C05-C04-C07-C08
2	B	1301	NAD	O4B-C4B-C5B-O5B
3	A	302	IDN	C03-C04-C07-C08
3	A	302	IDN	C07-C08-C09-O10
3	B	1302	IDN	C07-C08-C09-O10
3	B	1302	IDN	C03-C04-C07-C08
2	A	301	NAD	O4B-C4B-C5B-O5B
3	A	302	IDN	C07-C08-C09-N11
3	B	1302	IDN	C07-C08-C09-N11
3	B	1302	IDN	C05-C04-C07-C08
2	B	1301	NAD	C3B-C4B-C5B-O5B
2	B	1301	NAD	PA-O3-PN-O2N
2	B	1301	NAD	C5B-O5B-PA-O1A
2	A	301	NAD	C2D-C1D-N1N-C6N
2	B	1301	NAD	O4D-C1D-N1N-C6N
2	B	1301	NAD	PA-O3-PN-O1N

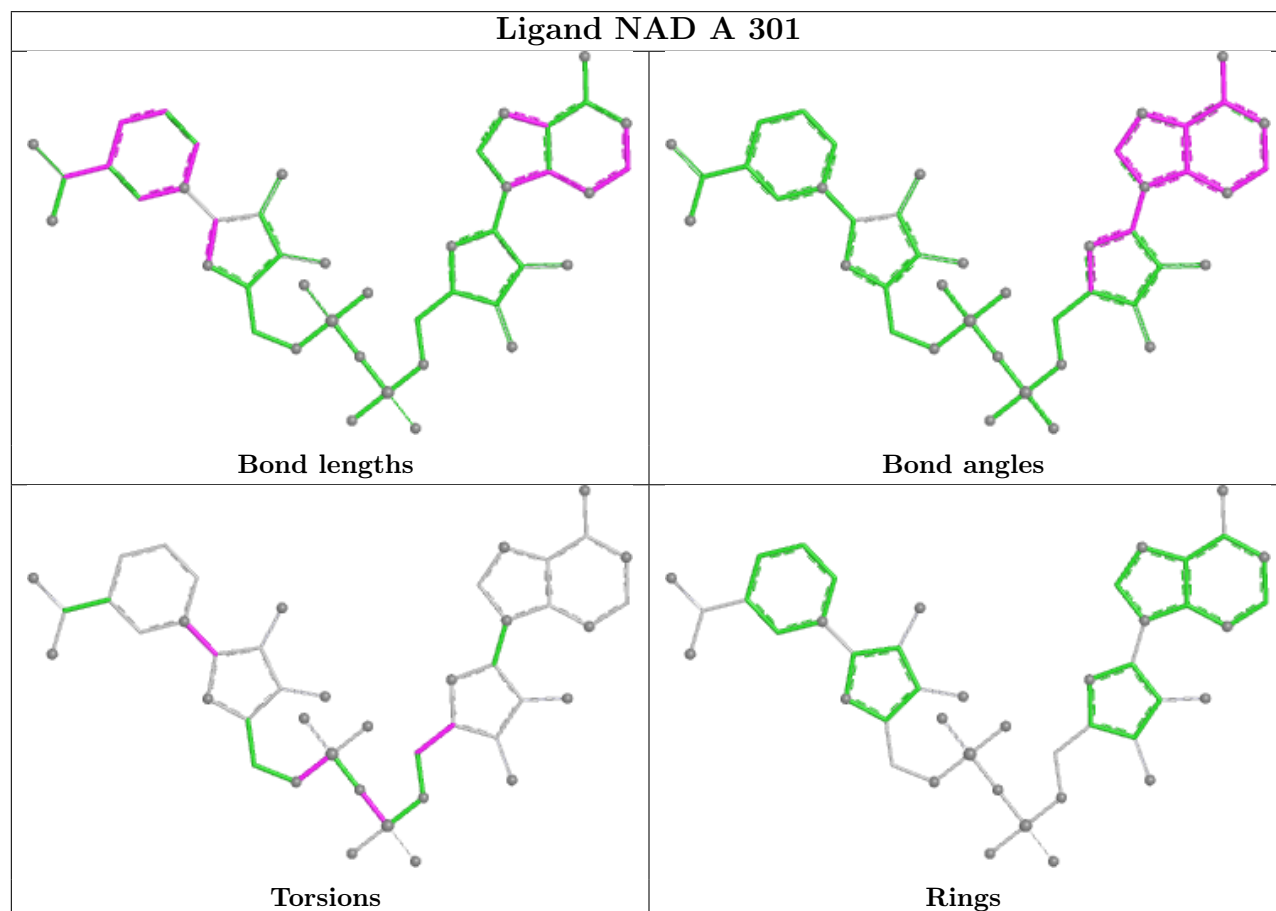
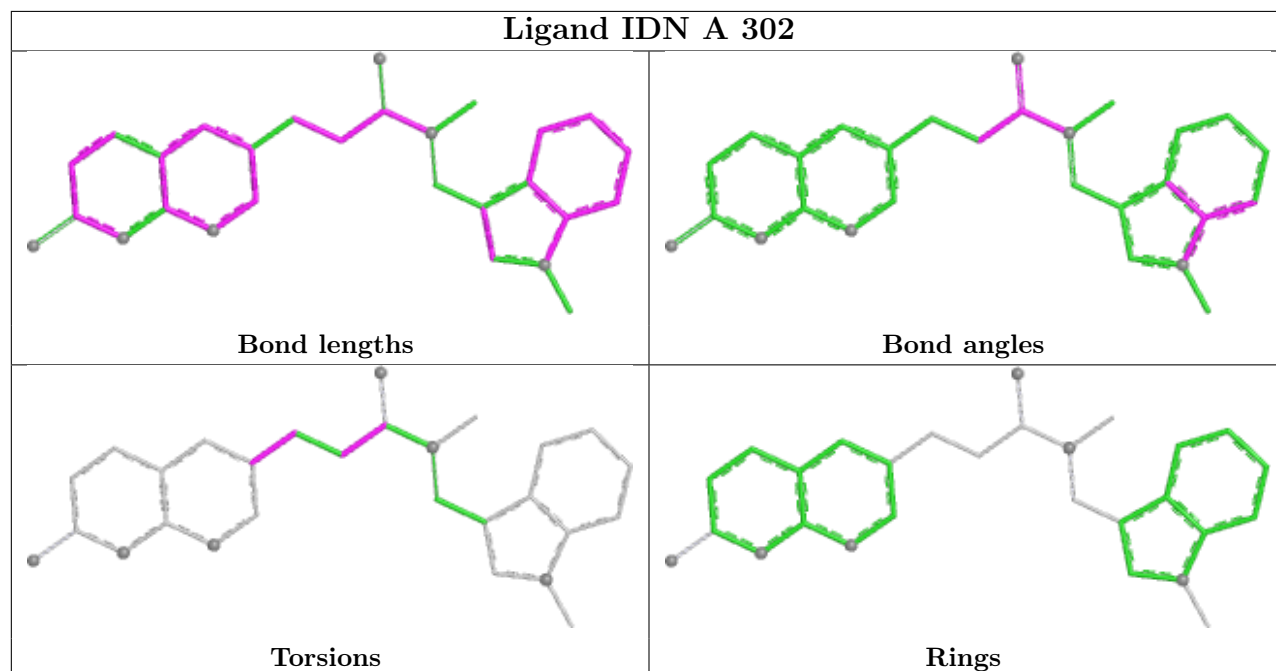
There are no ring outliers.

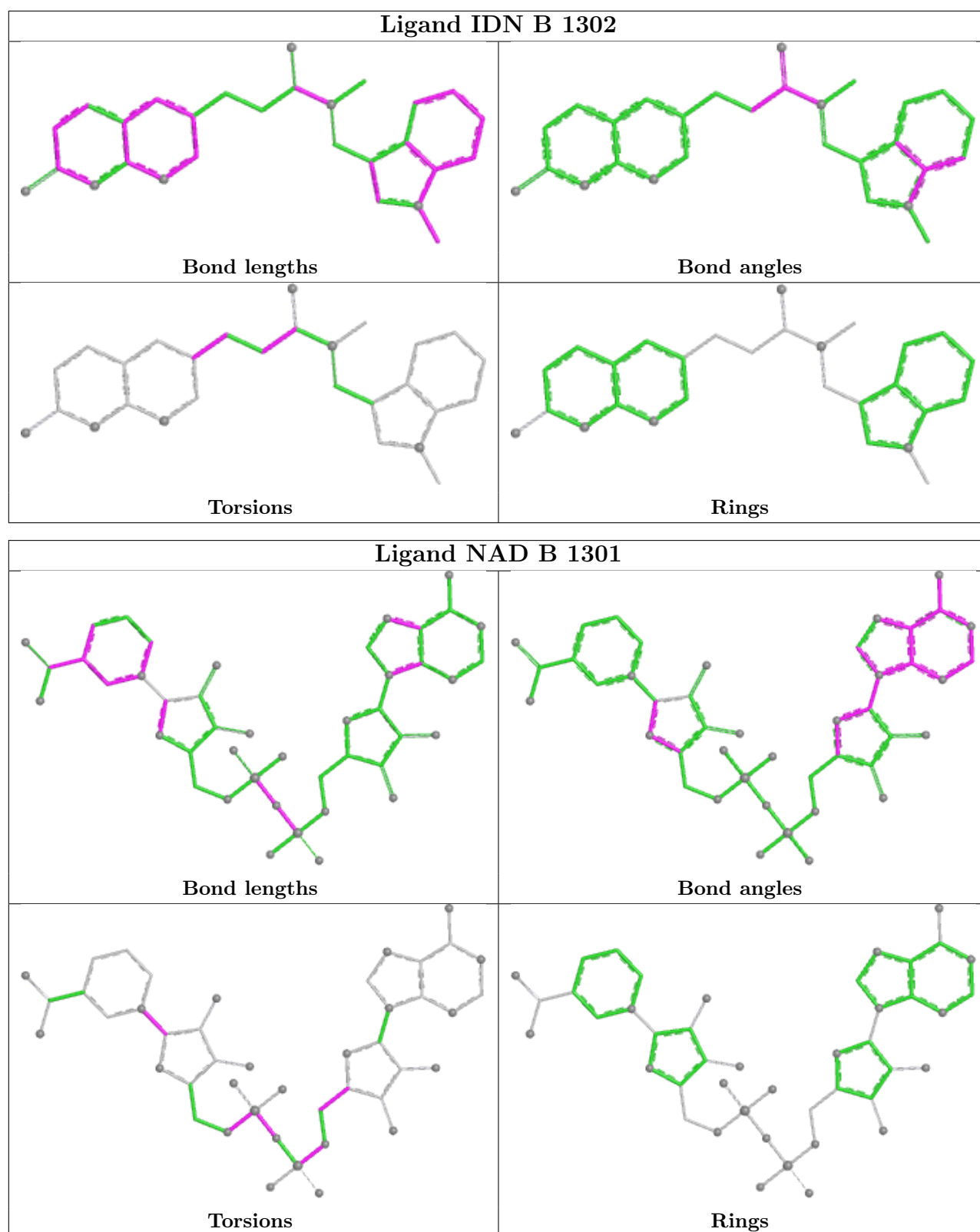
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	IDN	4	0
2	A	301	NAD	2	0
3	B	1302	IDN	4	0
2	B	1301	NAD	3	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 [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	258/262 (98%)	-0.02	11 (4%) 40 46	15, 28, 57, 85	0
1	B	258/262 (98%)	-0.12	8 (3%) 51 58	14, 26, 57, 91	0
All	All	516/524 (98%)	-0.07	19 (3%) 45 51	14, 27, 57, 91	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1200	ILE	4.4
1	B	1196	ALA	4.3
1	B	1195	LEU	4.0
1	A	259	LEU	3.8
1	A	200	ILE	3.5
1	B	1199	GLY	3.4
1	A	202	ASP	3.3
1	B	1198	SER	3.1
1	A	199	GLY	3.1
1	A	47	ARG	3.0
1	A	77	GLU	2.8
1	A	197	ALA	2.8
1	B	1197	ALA	2.6
1	B	1203	PHE	2.4
1	A	203	PHE	2.3
1	B	1098	ASP	2.3
1	A	196	ALA	2.2
1	A	98	ASP	2.2
1	A	198	SER	2.2

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](#)

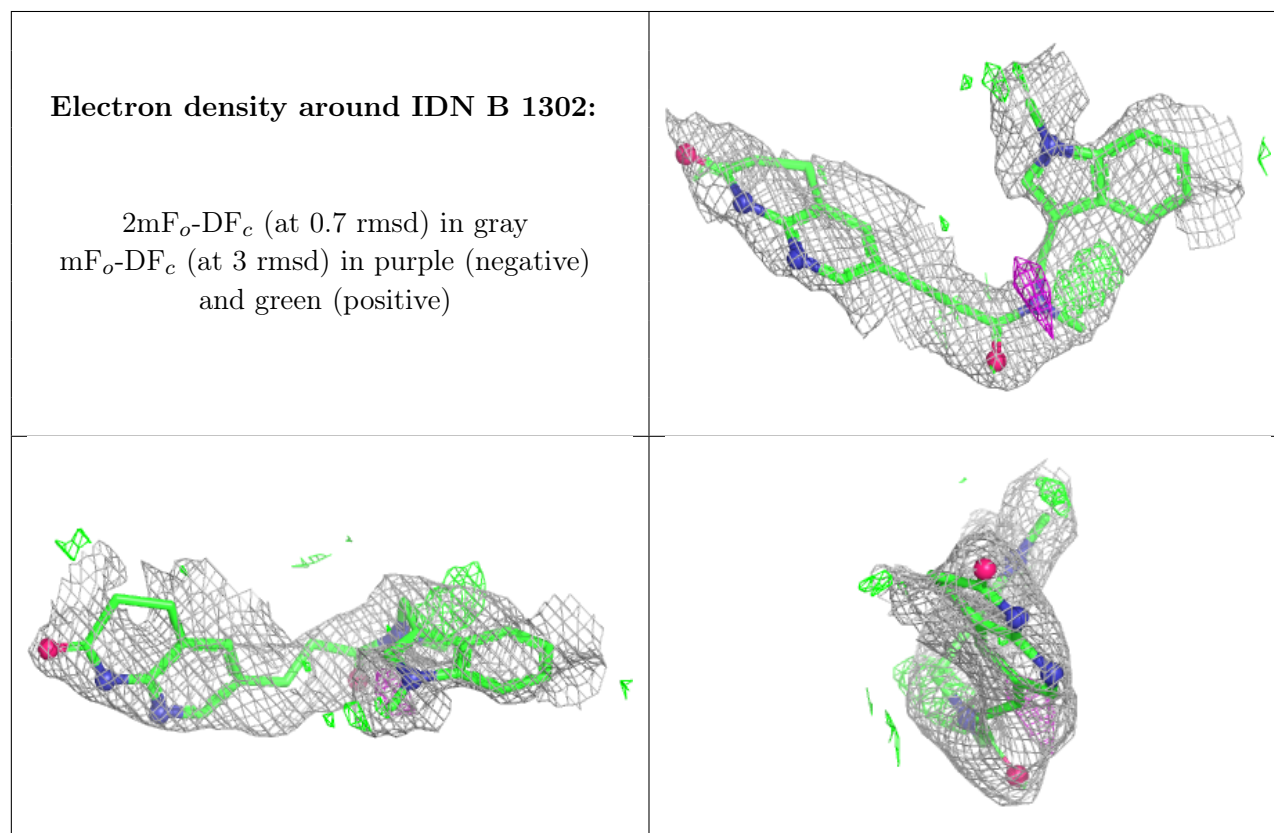
There are no oligosaccharides in this entry.

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.

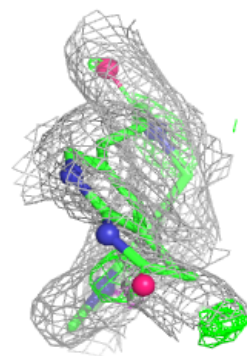
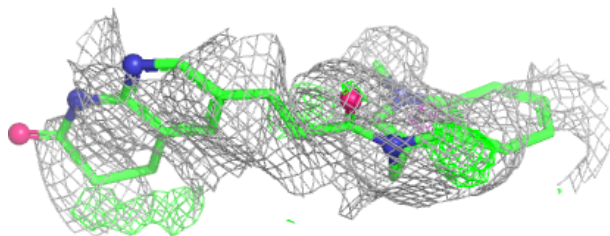
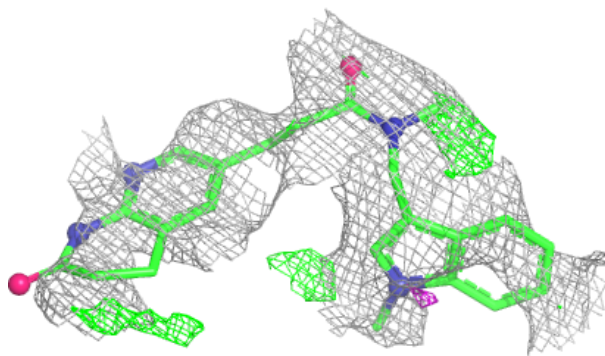
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IDN	B	1302	28/28	0.76	0.18	78,80,83,84	0
3	IDN	A	302	28/28	0.80	0.18	83,87,88,88	0
2	NAD	A	301	44/44	0.92	0.09	35,39,45,48	0
2	NAD	B	1301	44/44	0.93	0.09	34,39,46,49	0
4	SO4	B	1303	5/5	0.98	0.07	45,47,47,47	0

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.

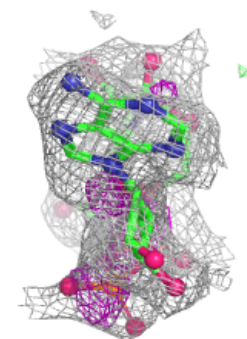
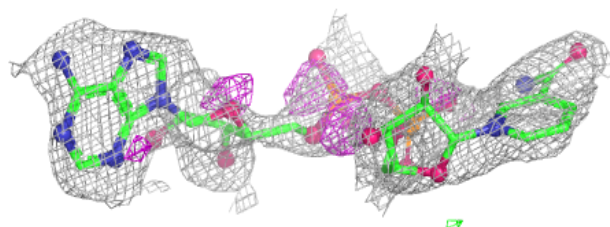
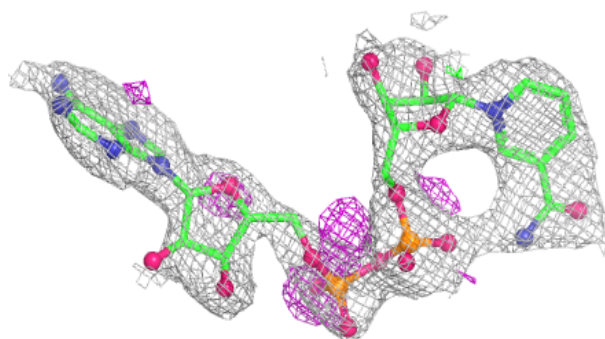


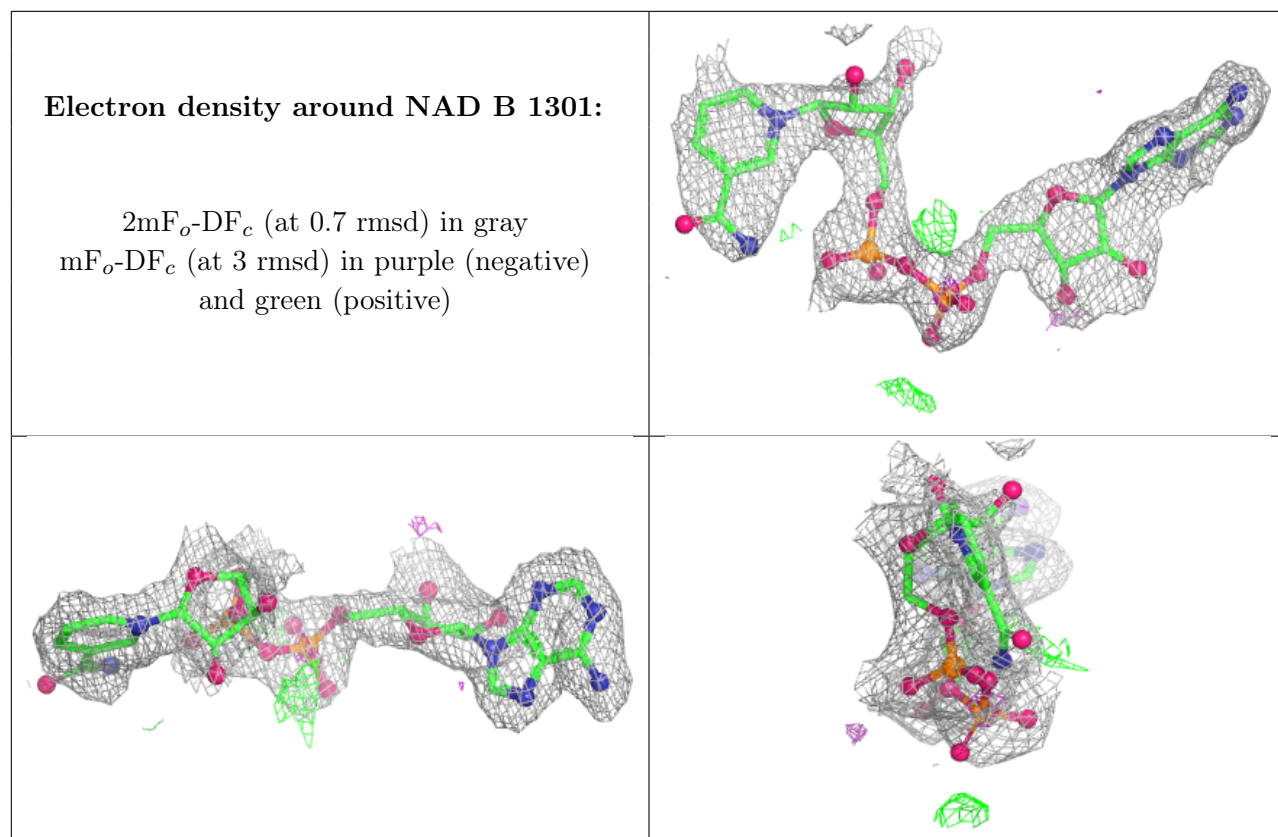
Electron density around IDN A 302:

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

**Electron density around NAD A 301:**

$2mF_o-DF_c$ (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.