



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2026 – 10:54 PM EDT

PDB ID : 1IFX / pdb_00001ifx
Title : CRYSTAL STRUCTURE OF NH₃-DEPENDENT NAD⁺ SYNTHETASE
FROM BACILLUS SUBTILIS COMPLEXED WITH TWO MOLECULES
DEAMIDO-NAD
Authors : Devedjiev, Y.; Symersky, J.; Singh, R.; Brouillette, W.; Muccio, D.; Jedrzejas,
M.; Brouillette, C.; DeLucas, L.
Deposited on : 2001-04-13
Resolution : 2.25 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)
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

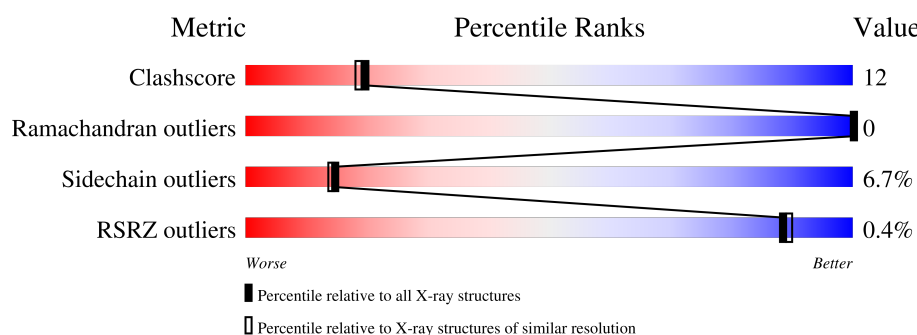
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	271	
1	B	271	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DND	A	8000	X	-	-	-
2	DND	B	7000	X	-	-	-

2 Entry composition [i](#)

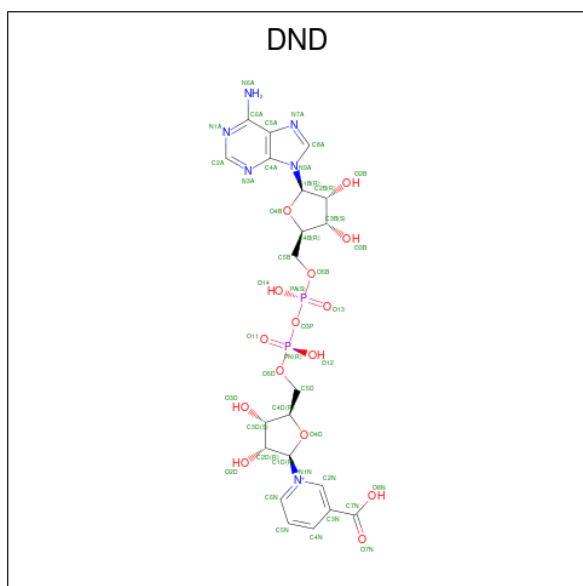
There are 3 unique types of molecules in this entry. The entry contains 4174 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NH(3)-DEPENDENT NAD(+) SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1927	1217	332	373	5			
1	B	245	Total	C	N	O	S	0	0	0
			1927	1217	332	373	5			

- Molecule 2 is NICOTINIC ACID ADENINE DINUCLEOTIDE (CCD ID: DND) (formula: $C_{21}H_{27}N_6O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	6	15	2		

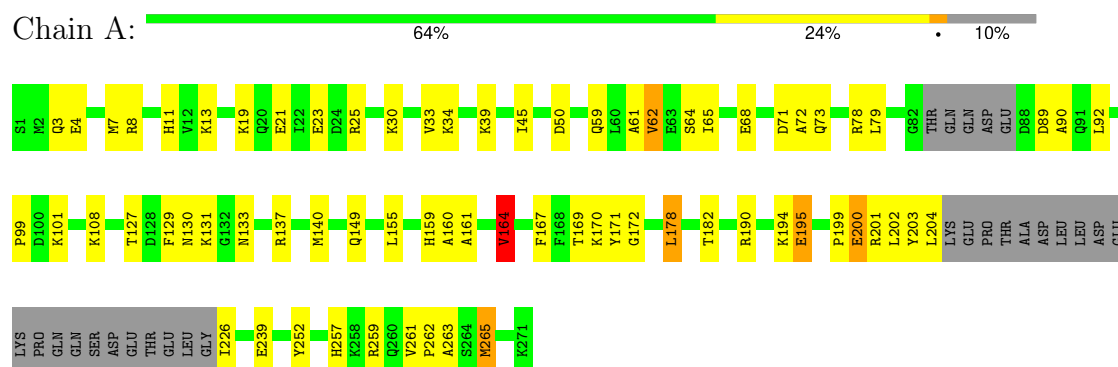
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total 117	O 117	0	0
3	B	115	Total 115	O 115	0	0

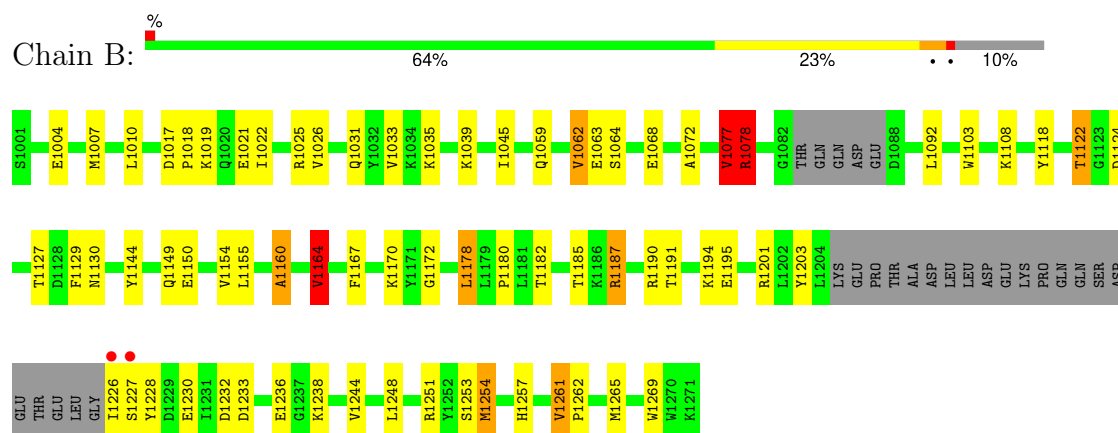
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NH(3)-DEPENDENT NAD(+) SYNTHETASE



• Molecule 1: NH(3)-DEPENDENT NAD(+) SYNTHETASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.06Å 86.09Å 61.08Å 90.00° 111.18° 90.00°	Depositor
Resolution (Å)	8.00 – 2.25 8.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (8.00-2.25) 97.3 (8.00-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.25Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.195 , 0.297 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 89.3	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	0.94	EDS
Total number of atoms	4174	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% 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: DND

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	0.79	1/1959 (0.1%)	1.12	10/2629 (0.4%)
1	B	0.81	1/1959 (0.1%)	1.16	10/2629 (0.4%)
All	All	0.80	2/3918 (0.1%)	1.14	20/5258 (0.4%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	MET	SD-CE	-5.94	1.64	1.79
1	B	1154	VAL	CA-CB	5.20	1.60	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	VAL	CB-CA-C	-8.55	100.59	112.14
1	B	1160	ALA	N-CA-C	8.36	121.14	111.11
1	B	1017	ASP	N-CA-C	-6.67	96.36	109.10
1	B	1164	VAL	CB-CA-C	-6.22	103.74	112.14
1	B	1077	VAL	CB-CA-C	-6.21	101.36	110.62
1	B	1108	LYS	N-CA-C	5.83	117.63	111.28
1	A	131	LYS	N-CA-C	-5.71	105.13	111.36
1	A	200	GLU	N-CA-C	5.71	118.27	111.71
1	B	1180	PRO	N-CA-C	5.67	121.01	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1150	GLU	N-CA-C	5.64	120.32	113.38
1	A	50	ASP	N-CA-C	5.60	117.06	111.07
1	B	1026	VAL	N-CA-C	-5.51	105.13	110.42
1	A	3	GLN	N-CA-C	-5.50	105.18	111.07
1	A	263	ALA	N-CA-C	5.38	118.24	110.28
1	A	108	LYS	N-CA-C	5.37	116.81	111.07
1	B	1172	GLY	N-CA-C	-5.23	100.79	113.18
1	A	13	LYS	CA-C-N	-5.15	113.73	119.19
1	A	13	LYS	C-N-CA	-5.15	113.73	119.19
1	A	11	HIS	N-CA-C	5.11	118.78	112.24
1	B	1078	ARG	N-CA-C	-5.05	101.47	109.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1144	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	1927	0	1921	46	0
1	B	1927	0	1918	54	0
2	A	44	0	23	5	0
2	B	44	0	21	4	0
3	A	117	0	0	0	0
3	B	115	0	0	2	0
All	All	4174	0	3883	90	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 12.

All (90) 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:1191:THR:HA	1:B:1194:LYS:HE2	1.42	0.99
1:B:1118:TYR:O	1:B:1122:THR:HB	1.84	0.77
1:B:1031:GLN:O	1:B:1035:LYS:HD3	1.86	0.75
1:A:149:GLN:HE21	1:B:1130:ASN:HD22	1.32	0.74
1:B:1227:SER:HB3	1:B:1230:GLU:HG3	1.69	0.73
1:B:1021:GLU:O	1:B:1025:ARG:HG3	1.91	0.70
1:A:149:GLN:NE2	1:B:1130:ASN:HD22	1.91	0.69
1:A:78:ARG:HD3	1:A:90:ALA:HB1	1.74	0.69
1:A:21:GLU:O	1:A:25:ARG:HG3	1.96	0.66
1:A:155:LEU:HD23	1:A:178:LEU:HD13	1.77	0.64
1:A:261:VAL:HG13	1:A:262:PRO:HD2	1.80	0.64
1:B:1025:ARG:NH2	1:B:1182:THR:O	2.29	0.63
1:B:1257:HIS:HE1	3:B:6099:HOH:O	1.81	0.63
1:A:199:PRO:HD2	1:A:202:LEU:HD12	1.80	0.63
1:B:1077:VAL:HG13	1:B:1103:TRP:HB2	1.79	0.63
1:A:149:GLN:HE21	1:B:1130:ASN:ND2	1.96	0.63
1:A:45:ILE:O	1:A:78:ARG:NH1	2.31	0.62
1:A:149:GLN:HE22	1:B:1127:THR:H	1.46	0.62
1:B:1155:LEU:HD23	1:B:1178:LEU:HD13	1.82	0.61
1:A:19:LYS:HE2	1:A:195:GLU:OE1	2.01	0.60
1:A:73:GLN:OE1	1:A:101:LYS:HE3	2.01	0.60
1:A:133:ASN:OD1	2:A:8000:DND:H3	2.01	0.60
1:B:1078:ARG:HA	1:B:1078:ARG:HE	1.67	0.59
1:B:1059:GLN:O	1:B:1063:GLU:HG3	2.04	0.58
1:B:1167:PHE:CD2	2:B:7000:DND:H13	2.38	0.58
1:B:1190:ARG:HG3	1:B:1203:TYR:HB2	1.85	0.56
1:B:1122:THR:HG22	1:B:1124:ASP:H	1.71	0.56
1:B:1226:ILE:CD1	1:B:1244:VAL:HG13	2.36	0.56
1:B:1187:ARG:HD2	1:B:1236:GLU:OE2	2.06	0.56
1:A:130:ASN:HD22	1:B:1149:GLN:HE21	1.54	0.55
1:B:1129:PHE:HE2	2:B:7000:DND:O11	1.89	0.55
1:A:4:GLU:HG2	1:A:8:ARG:HH21	1.73	0.54
1:A:64:SER:O	1:A:68:GLU:HG3	2.07	0.54
1:B:1160:ALA:O	1:B:1164:VAL:HG22	2.08	0.54
1:A:30:LYS:O	1:A:34:LYS:HG3	2.07	0.54
1:A:78:ARG:NH1	1:A:79:LEU:H	2.06	0.54
1:A:265:MET:HE3	3:B:6053:HOH:O	2.07	0.54
1:A:25:ARG:NH2	1:A:182:THR:O	2.42	0.53
1:A:129:PHE:CZ	2:A:8000:DND:H2	2.45	0.51
1:A:130:ASN:HD22	1:B:1149:GLN:NE2	2.08	0.51
1:A:130:ASN:ND2	1:B:1149:GLN:HE21	2.08	0.51
1:B:1129:PHE:CE2	2:B:7000:DND:O11	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1257:HIS:HA	1:B:1269:TRP:CH2	2.45	0.51
1:A:160:ALA:O	1:A:164:VAL:HG22	2.10	0.51
1:B:1190:ARG:O	1:B:1194:LYS:HG3	2.11	0.51
1:A:59:GLN:NE2	1:A:99:PRO:HA	2.26	0.50
1:B:1062:VAL:HG22	1:B:1072:ALA:HB1	1.92	0.50
1:A:127:THR:H	1:B:1149:GLN:HE22	1.58	0.50
1:A:159:HIS:CD2	1:A:161:ALA:HB3	2.48	0.49
1:B:1122:THR:HG22	1:B:1124:ASP:N	2.27	0.49
1:A:252:TYR:O	1:A:259:ARG:NH2	2.46	0.49
1:B:1064:SER:O	1:B:1068:GLU:HG3	2.13	0.49
1:B:1170:LYS:NZ	1:B:1257:HIS:HD2	2.11	0.49
1:B:1254:MET:HB3	1:B:1254:MET:HE2	1.78	0.48
1:B:1045:ILE:O	1:B:1078:ARG:NE	2.48	0.47
1:B:1227:SER:HB3	1:B:1230:GLU:CG	2.40	0.47
1:B:1261:VAL:HG13	1:B:1262:PRO:HD2	1.97	0.47
1:A:140:MET:HE2	1:A:171:TYR:O	2.15	0.46
1:A:265:MET:HE1	1:B:1025:ARG:HG2	1.98	0.46
1:B:1018:PRO:O	1:B:1022:ILE:HG13	2.16	0.45
1:A:169:THR:OG1	2:A:8000:DND:H10	2.16	0.45
1:B:1018:PRO:HB3	1:B:1191:THR:HG22	1.97	0.45
1:B:1201:ARG:HD2	1:B:1201:ARG:O	2.16	0.45
1:B:1226:ILE:HD12	1:B:1244:VAL:HG13	1.98	0.45
1:A:167:PHE:CE1	2:A:8000:DND:H7	2.52	0.44
1:B:1185:THR:HB	1:B:1232:ASP:OD1	2.16	0.44
1:B:1233:ASP:OD2	1:B:1238:LYS:HD2	2.18	0.44
1:B:1078:ARG:HA	1:B:1078:ARG:NE	2.32	0.44
1:A:190:ARG:O	1:A:194:LYS:HG3	2.18	0.44
1:A:89:ASP:OD1	1:A:201:ARG:HD2	2.18	0.43
1:B:1251:ARG:HA	1:B:1251:ARG:HD2	1.67	0.43
1:B:1248:LEU:HD23	1:B:1248:LEU:HA	1.82	0.43
1:B:1167:PHE:CE2	2:B:7000:DND:H13	2.53	0.43
1:A:129:PHE:HZ	2:A:8000:DND:O11	2.02	0.43
1:A:61:ALA:O	1:A:65:ILE:HG13	2.19	0.42
1:A:78:ARG:CD	1:A:90:ALA:HB1	2.45	0.42
1:B:1010:LEU:HD11	1:B:1164:VAL:HG13	2.01	0.42
1:A:21:GLU:OE1	1:A:25:ARG:NH1	2.52	0.42
1:B:1004:GLU:HA	1:B:1007:MET:HE2	2.00	0.42
1:B:1194:LYS:HG2	1:B:1203:TYR:CZ	2.55	0.42
1:A:78:ARG:HA	1:A:78:ARG:HD2	1.79	0.42
1:A:170:LYS:NZ	1:A:257:HIS:HD2	2.18	0.41
1:A:200:GLU:HA	1:A:203:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLU:HG3	1:A:204:LEU:HD12	2.02	0.41
1:B:1039:LYS:HA	1:B:1039:LYS:HD3	1.88	0.41
1:A:39:LYS:O	1:A:72:ALA:HA	2.21	0.41
1:A:149:GLN:NE2	1:B:1127:THR:H	2.17	0.41
1:A:137:ARG:HA	1:A:172:GLY:HA2	2.03	0.41
1:B:1227:SER:O	1:B:1230:GLU:HB2	2.21	0.40
1:A:62:VAL:HG22	1:A:72:ALA:HB1	2.03	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	239/271 (88%)	237 (99%)	2 (1%)	0	100	100
1	B	239/271 (88%)	238 (100%)	1 (0%)	0	100	100
All	All	478/542 (88%)	475 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	202/226 (89%)	191 (95%)	11 (5%)	20	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	202/226 (89%)	186 (92%)	16 (8%)	11	9
All	All	404/452 (89%)	377 (93%)	27 (7%)	15	14

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	MET
1	A	23	GLU
1	A	33	VAL
1	A	62	VAL
1	A	71	ASP
1	A	92	LEU
1	A	164	VAL
1	A	178	LEU
1	A	195	GLU
1	A	226	ILE
1	A	239	GLU
1	B	1019	LYS
1	B	1033	VAL
1	B	1062	VAL
1	B	1077	VAL
1	B	1078	ARG
1	B	1092	LEU
1	B	1122	THR
1	B	1164	VAL
1	B	1178	LEU
1	B	1187	ARG
1	B	1195	GLU
1	B	1228	TYR
1	B	1253	SER
1	B	1254	MET
1	B	1261	VAL
1	B	1265	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	20	GLN
1	A	59	GLN
1	A	81	HIS

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Mol	Chain	Res	Type
1	A	117	GLN
1	A	130	ASN
1	A	143	GLN
1	A	149	GLN
1	A	159	HIS
1	A	257	HIS
1	B	1011	HIS
1	B	1020	GLN
1	B	1059	GLN
1	B	1073	GLN
1	B	1117	GLN
1	B	1149	GLN
1	B	1159	HIS
1	B	1257	HIS

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	DND	B	7000	-	46,48,48	1.50	5 (10%)	64,73,73	3.32	30 (46%)
2	DND	A	8000	-	46,48,48	1.56	9 (19%)	64,73,73	3.51	28 (43%)

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	DND	B	7000	-	3/3/11/11	5/30/62/62	0/5/5/5
2	DND	A	8000	-	2/2/11/11	14/30/62/62	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7000	DND	C2N-N1N	5.85	1.41	1.35
2	A	8000	DND	C2N-N1N	4.81	1.40	1.35
2	A	8000	DND	PN-O3P	3.88	1.63	1.59
2	B	7000	DND	C5A-N7A	-3.46	1.32	1.39
2	B	7000	DND	C6N-N1N	3.40	1.43	1.35
2	A	8000	DND	C5A-N7A	-3.29	1.33	1.39
2	A	8000	DND	C3N-C7N	3.16	1.56	1.49
2	A	8000	DND	C6N-N1N	2.97	1.42	1.35
2	B	7000	DND	O8N-C7N	-2.46	1.23	1.30
2	B	7000	DND	C4A-N9A	-2.22	1.33	1.37
2	A	8000	DND	PA-O14	-2.20	1.45	1.55
2	A	8000	DND	C4N-C3N	2.11	1.42	1.39
2	A	8000	DND	PA-O3P	2.10	1.61	1.59
2	A	8000	DND	C4A-N9A	-2.09	1.33	1.37

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	8000	DND	C4D-O4D-C1D	-16.12	95.16	109.92
2	B	7000	DND	C4D-O4D-C1D	-11.42	99.47	109.92
2	B	7000	DND	O3B-C3B-C4B	7.94	133.90	111.08
2	B	7000	DND	O2B-C2B-C1B	7.43	135.68	110.10
2	B	7000	DND	O3D-C3D-C4D	7.25	131.91	111.08
2	A	8000	DND	N3A-C4A-N9A	6.88	138.88	127.17
2	A	8000	DND	C5A-C4A-N3A	-6.87	117.26	126.72
2	A	8000	DND	O3B-C3B-C4B	6.67	130.24	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	8000	DND	O5D-C5D-C4D	-6.06	88.36	108.99
2	A	8000	DND	O3D-C3D-C4D	5.50	126.88	111.08
2	A	8000	DND	C6A-C5A-N7A	-5.39	121.69	132.09
2	B	7000	DND	N3A-C4A-N9A	5.31	136.19	127.17
2	B	7000	DND	C5A-C4A-N3A	-5.29	119.43	126.72
2	B	7000	DND	C2B-C1B-N9A	5.18	126.17	113.30
2	B	7000	DND	N1A-C2A-N3A	-5.14	120.80	128.58
2	B	7000	DND	O5D-C5D-C4D	-5.06	91.76	108.99
2	A	8000	DND	O2B-C2B-C1B	5.04	127.47	110.10
2	A	8000	DND	O4D-C4D-C5D	4.85	124.87	109.33
2	A	8000	DND	C6A-C5A-C4A	4.83	123.77	117.18
2	A	8000	DND	C2B-C1B-N9A	4.51	124.51	113.30
2	B	7000	DND	C6A-C5A-N7A	-4.35	123.71	132.09
2	A	8000	DND	O4B-C1B-N9A	4.15	116.06	108.09
2	B	7000	DND	O2D-C2D-C3D	4.06	124.85	111.82
2	B	7000	DND	O12-PN-O3P	3.99	118.05	107.27
2	B	7000	DND	O4D-C4D-C3D	3.96	113.01	105.15
2	B	7000	DND	O3P-PN-O11	-3.78	99.32	110.70
2	A	8000	DND	C4B-O4B-C1B	-3.71	101.28	109.47
2	B	7000	DND	C6A-C5A-C4A	3.70	122.23	117.18
2	A	8000	DND	N1A-C2A-N3A	-3.69	122.99	128.58
2	A	8000	DND	C5B-C4B-C3B	3.66	128.40	115.21
2	B	7000	DND	O4D-C4D-C5D	3.61	120.90	109.33
2	A	8000	DND	O4B-C4B-C3B	3.55	112.21	105.15
2	B	7000	DND	C2A-N1A-C6A	3.53	124.53	118.73
2	A	8000	DND	O3D-C3D-C2D	3.33	122.49	111.82
2	B	7000	DND	C5B-C4B-C3B	3.26	126.94	115.21
2	B	7000	DND	O4B-C4B-C3B	3.25	111.60	105.15
2	A	8000	DND	C2A-N3A-C4A	3.23	119.73	111.83
2	B	7000	DND	C6N-N1N-C2N	-3.22	119.14	121.88
2	A	8000	DND	C5N-C4N-C3N	3.10	123.41	120.36
2	B	7000	DND	O4B-C4B-C5B	3.10	119.26	109.33
2	B	7000	DND	C5D-C4D-C3D	2.98	125.94	115.21
2	B	7000	DND	C4A-C5A-N7A	2.96	113.97	110.58
2	A	8000	DND	O4D-C4D-C3D	2.95	111.01	105.15
2	B	7000	DND	C2A-N3A-C4A	2.92	118.97	111.83
2	B	7000	DND	O3P-PA-O13	-2.85	102.13	110.70
2	B	7000	DND	O3B-C3B-C2B	2.76	120.66	111.82
2	B	7000	DND	C2D-C3D-C4D	-2.72	97.36	102.61
2	B	7000	DND	C4B-O4B-C1B	-2.69	103.53	109.47
2	A	8000	DND	C4A-C5A-N7A	2.66	113.62	110.58
2	A	8000	DND	O12-PN-O3P	2.60	114.30	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	8000	DND	C5A-C4A-N9A	-2.45	103.14	105.81
2	A	8000	DND	C5D-C4D-C3D	2.43	123.96	115.21
2	A	8000	DND	C4A-N9A-C8A	2.36	108.22	105.74
2	A	8000	DND	O7N-C7N-C3N	-2.29	115.45	121.46
2	B	7000	DND	O3D-C3D-C2D	2.23	118.98	111.82
2	B	7000	DND	O5D-PN-O11	2.23	117.76	108.94
2	A	8000	DND	N6A-C6A-N1A	2.22	123.31	118.38
2	A	8000	DND	C1B-N9A-C8A	-2.18	122.26	127.09

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	8000	DND	C4D
2	A	8000	DND	C3D
2	B	7000	DND	C4D
2	B	7000	DND	C3D
2	B	7000	DND	C3B

All (19) torsion outliers are listed below:

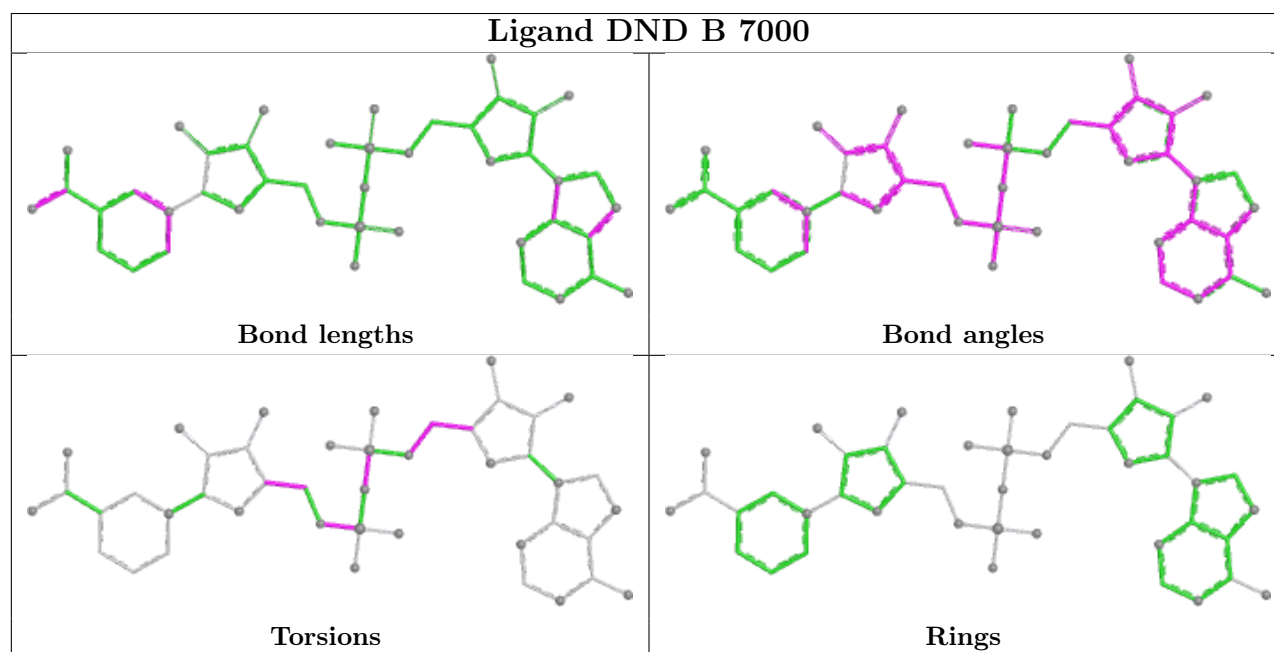
Mol	Chain	Res	Type	Atoms
2	A	8000	DND	C5D-O5D-PN-O11
2	A	8000	DND	C5D-O5D-PN-O3P
2	A	8000	DND	C2D-C1D-N1N-C6N
2	A	8000	DND	C2D-C1D-N1N-C2N
2	B	7000	DND	PN-O3P-PA-O5B
2	B	7000	DND	C3B-C4B-C5B-O5B
2	A	8000	DND	C4N-C3N-C7N-O8N
2	A	8000	DND	C3D-C4D-C5D-O5D
2	A	8000	DND	C3B-C4B-C5B-O5B
2	B	7000	DND	C3D-C4D-C5D-O5D
2	A	8000	DND	C4N-C3N-C7N-O7N
2	A	8000	DND	O4D-C4D-C5D-O5D
2	A	8000	DND	C5D-O5D-PN-O12
2	A	8000	DND	C5B-O5B-PA-O13
2	B	7000	DND	C5D-O5D-PN-O11
2	B	7000	DND	C4B-C5B-O5B-PA
2	A	8000	DND	C4B-C5B-O5B-PA
2	A	8000	DND	PA-O3P-PN-O12
2	A	8000	DND	PA-O3P-PN-O11

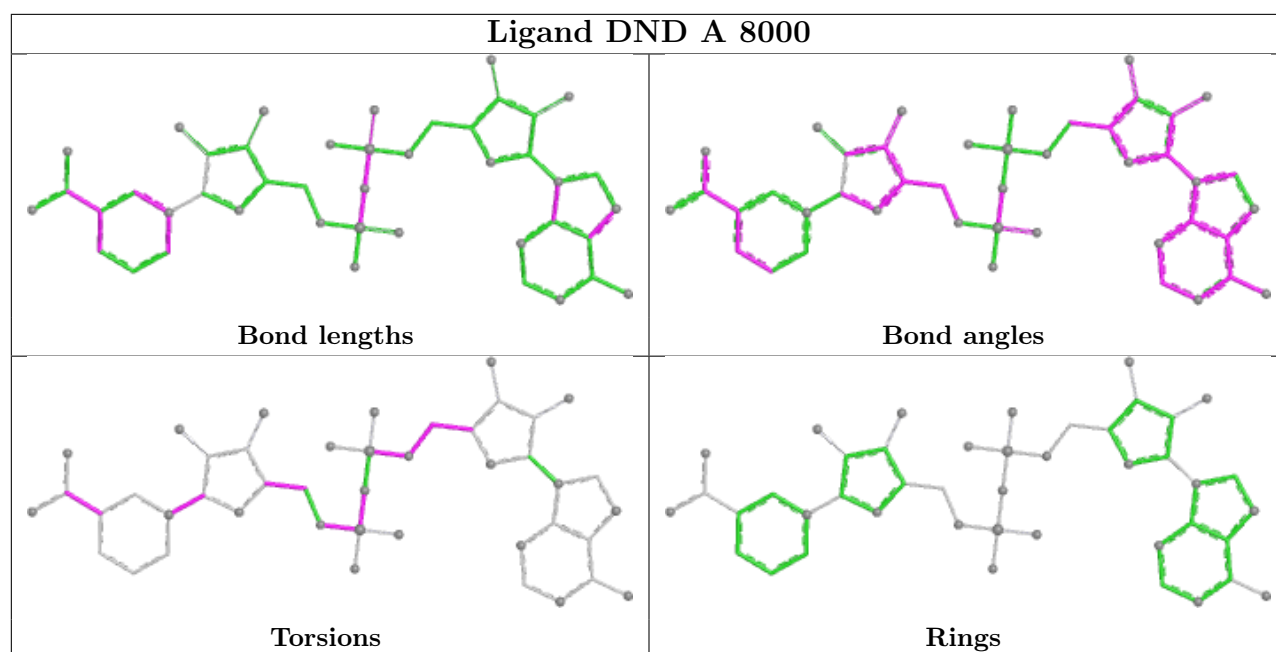
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	7000	DND	4	0
2	A	8000	DND	5	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	245/271 (90%)	-0.72	0	100 100	6, 18, 38, 49	0
1	B	245/271 (90%)	-0.60	2 (0%)	82 84	10, 20, 47, 64	0
All	All	490/542 (90%)	-0.66	2 (0%)	88 89	6, 19, 42, 64	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1227	SER	2.7
1	B	1226	ILE	2.4

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](#)

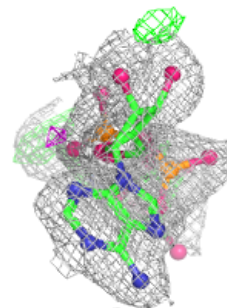
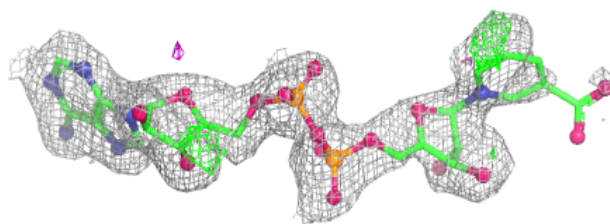
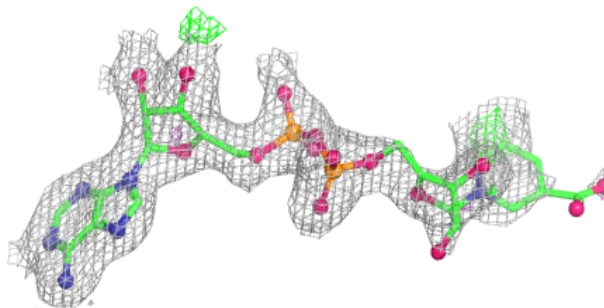
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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	DND	A	8000	44/44	0.94	0.08	14,28,71,77	0
2	DND	B	7000	44/44	0.95	0.08	16,31,78,79	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.

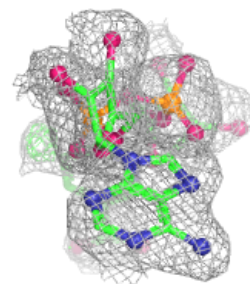
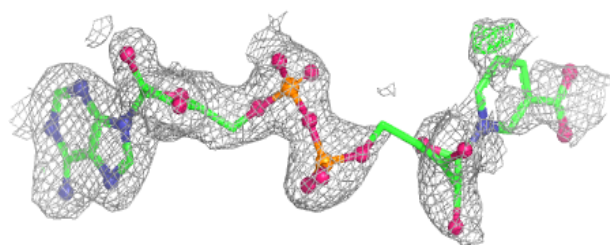
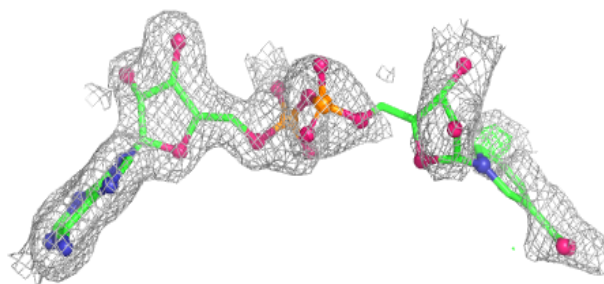
Electron density around DND A 8000:

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



Electron density around DND B 7000:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.