WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2024 – 07:54 PM EST

PDB ID	:	1KAQ
Title	:	Structure of Bacillus subtilis Nicotinic Acid Mononucleotide Adenylyl Transferase
Authors	:	Olland, A.M.; Underwood, K.W.; Czerwinski, R.M.; Lo, M.C.; Aulabaugh, A.; Bard, J.; Stahl, M.L.; Somers, W.S.; Sullivan, F.X.; Chopra, R.
Deposited on	:	2001-11-02
Resolution	:	3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

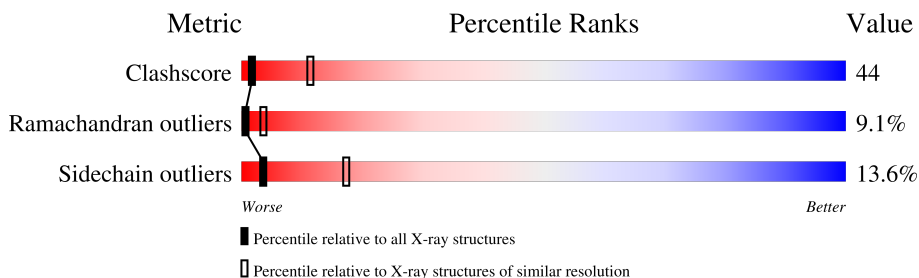|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 Å.

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

Metric	Percentile Ranks	Value
Clashscore		44
Ramachandran outliers		9.1%
Sidechain outliers		13.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	194	38% 45% 10% · ·
1	B	194	31% 46% 14% · ·
1	C	194	39% 44% 11% · ·
1	D	194	36% 48% 8% · ·
1	E	194	30% 50% 10% · 9%
1	F	194	24% 44% 12% 7% 14%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DND	A	601	X	-	-	-
2	DND	B	501	X	-	-	-
2	DND	C	401	X	-	-	-
2	DND	D	301	X	-	-	-
2	DND	E	201	X	-	-	-
2	DND	F	190	X	-	-	-

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 9268 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 NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1542	1010	246	280	6			
1	B	186	Total	C	N	O	S	0	0	0
			1542	1010	246	280	6			
1	C	186	Total	C	N	O	S	0	0	0
			1542	1010	246	280	6			
1	D	186	Total	C	N	O	S	0	0	0
			1542	1010	246	280	6			
1	E	176	Total	C	N	O	S	0	0	0
			1456	957	231	262	6			
1	F	167	Total	C	N	O	S	0	0	0
			1380	906	216	252	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP P54455
A	-3	MET	-	expression tag	UNP P54455
A	-2	PRO	-	expression tag	UNP P54455
A	-1	GLY	-	expression tag	UNP P54455
A	0	GLY	-	expression tag	UNP P54455
A	1	SER	MET	cloning artifact	UNP P54455
B	-4	HIS	-	expression tag	UNP P54455
B	-3	MET	-	expression tag	UNP P54455
B	-2	PRO	-	expression tag	UNP P54455
B	-1	GLY	-	expression tag	UNP P54455
B	0	GLY	-	expression tag	UNP P54455
B	1	SER	MET	cloning artifact	UNP P54455
C	-4	HIS	-	expression tag	UNP P54455
C	-3	MET	-	expression tag	UNP P54455
C	-2	PRO	-	expression tag	UNP P54455
C	-1	GLY	-	expression tag	UNP P54455
C	0	GLY	-	expression tag	UNP P54455

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	SER	MET	cloning artifact	UNP P54455
D	-4	HIS	-	expression tag	UNP P54455
D	-3	MET	-	expression tag	UNP P54455
D	-2	PRO	-	expression tag	UNP P54455
D	-1	GLY	-	expression tag	UNP P54455
D	0	GLY	-	expression tag	UNP P54455
D	1	SER	MET	cloning artifact	UNP P54455
E	-4	HIS	-	expression tag	UNP P54455
E	-3	MET	-	expression tag	UNP P54455
E	-2	PRO	-	expression tag	UNP P54455
E	-1	GLY	-	expression tag	UNP P54455
E	0	GLY	-	expression tag	UNP P54455
E	1	SER	MET	cloning artifact	UNP P54455
F	-4	HIS	-	expression tag	UNP P54455
F	-3	MET	-	expression tag	UNP P54455
F	-2	PRO	-	expression tag	UNP P54455
F	-1	GLY	-	expression tag	UNP P54455
F	0	GLY	-	expression tag	UNP P54455
F	1	SER	MET	cloning artifact	UNP P54455

- Molecule 2 is NICOTINIC ACID ADENINE DINUCLEOTIDE (three-letter code: DND) (formula: $C_{21}H_{27}N_6O_{15}P_2$).
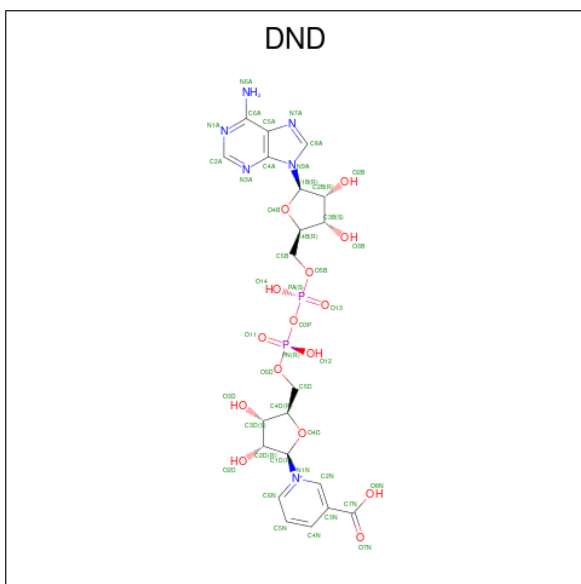
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	44	21	6	15	2	0	0

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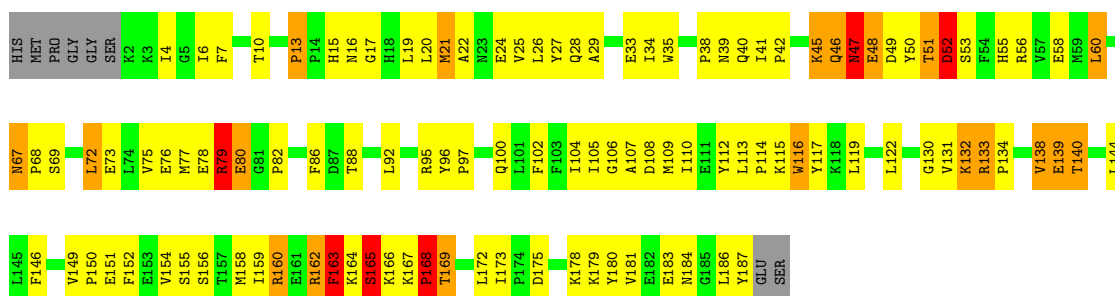| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	6	15	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	6	15	2		

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. 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. 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.
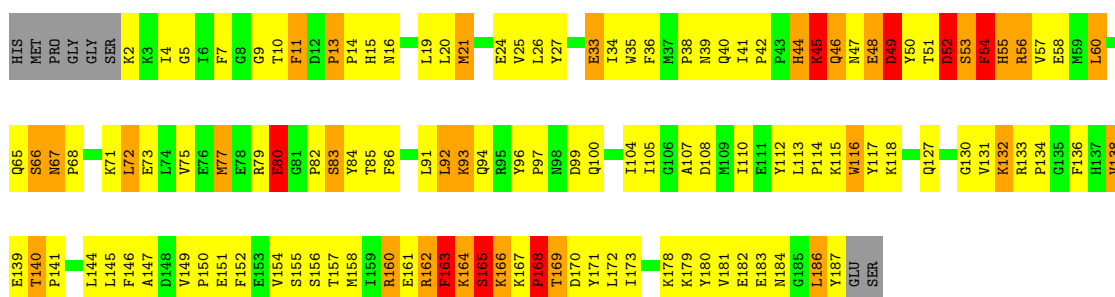
Note EDS was not executed.

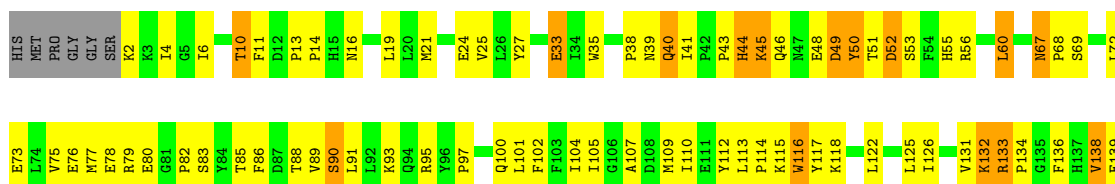• Molecule 1: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE

Chain A:

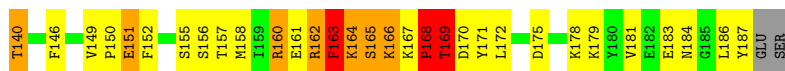• Molecule 1: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE

Chain B:

• Molecule 1: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE
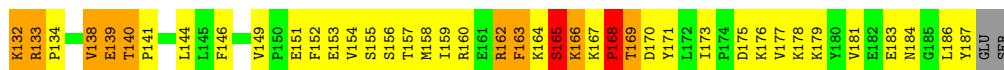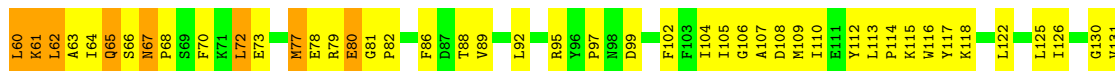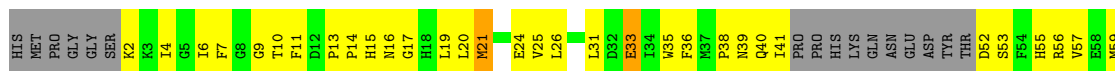
Chain C:

T140 F146 V149 P150 E151 F152 S155 S156 T157 M158 I159 R160 E161 R162 F163 K164 S165 K166 K167 P168 T169 D170 Y171 L172 D175 K178 K179 V180 V181 E182 E183 N184 G185 L186 Y187 GLU SER

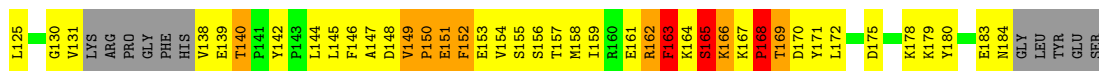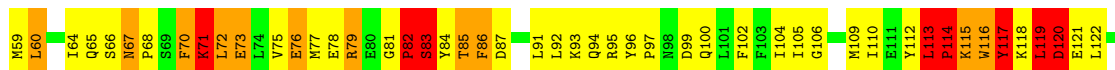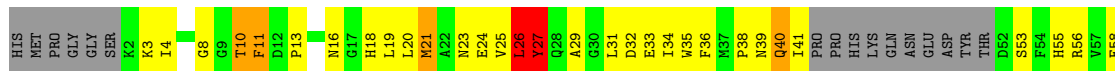• Molecule 1: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE

Chain D:

36%   48%   8% • •

HIS MET PRO GLY GLY SER K2 I6 F7 G8 G9 T10 F11 D12 P13 P14 H15 N16 L20 M21 A22 V25 L26 Y27 L31 D32 E33 F36 M37 P38 N39 Q40 I41 H44 K45 E48 D49 T51 Y50 D52 S53 F54 H55 R56 V57 E58 M59 L60 K61 Q65 S66 N67

P68 S69 L72 E73 L74 V75 E76 M77 E78 R79 E80 G81 P82 F86 D87 S90 L91 L92 K93 Q94 R95 Y96 P97 N98 D99 Q100 L101 I104 I105 G106 A107 D108 M109 I110 L113 W116 Y117 K118 L119 L122 L123 N124 L125 I126 V131 K132 R133 P134 G135 F136 H137 V138

E139 T140 P141 L144 L145 F146 A147 D148 V149 P150 E151 F152 E153 V154 S155 S156 T157 M158 I159 R160 E161 R162 F163 K164 S165 K166 K167 P168 T169 D170 Y171 L172 I173 P174 D175 K178 K179 V180 V181 E182 E183 N184 G185 L186 Y187 GLU SER

• Molecule 1: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE

Chain E:

30%   50%   10% • 9%

HIS MET PRO GLY GLY SER K2 K3 I4 G5 I6 F7 G8 G9 T10 F11 D12 P13 P14 H15 N16 G17 H18 L19 L20 M21 E24 V25 L26 L31 D32 E33 I34 W35 F36 M37 P38 N39 Q40 I41 PRO PRO HIS LYS GLN ASN GLU ASP TYR THR D52 S53 F54 H55 R56 V57 E58 M59

L60 K61 L62 A63 I64 Q65 S66 N67 P68 S69 F70 K71 L72 E73 M77 E78 R79 E80 G81 P82 F86 D87 T88 V89 L92 R95 Y96 P97 N98 D99 F102 F103 I104 I105 G106 A107 D108 M109 I110 E111 Y112 L113 P114 K115 W116 Y117 K118 L122 L125 I126 G130 V131

K132 R133 P134 V138 E139 T140 P141 L144 L145 F146 V149 P150 E151 F152 E153 V154 S155 S156 T157 M158 I159 R160 E161 R162 F163 K164 S165 K166 K167 P168 T169 D170 Y171 L172 I173 P174 D175 K176 V177 K178 K179 Y180 V181 E182 E183 N184 G185 L186 Y187 GLU SER

• Molecule 1: NICOTINATE-NUCLEOTIDE ADENYLYLTRANSFERASE

Chain F:

24%   44%   12% 7% 14%

HIS MET PRO GLY GLY SER K2 K3 I4 G8 G9 T10 F11 D12 P13 N16 G17 H18 L19 L20 M21 A22 N23 E24 V25 L26 Y27 Q28 A29 G30 L31 D32 E33 I34 W35 F36 M37 P38 N39 Q40 I41 PRO PRO HIS LYS GLN ASN GLU ASP TYR THR D52 S53 F54 H55 R56 V57 E58

M59 L60 I64 Q65 S66 N67 P68 S69 F70 K71 L72 E73 L74 V75 E76 M77 E78 R79 E80 G81 P82 S83 Y84 T85 F86 D87 L91 L92 K93 Q94 R95 Y96 P97 N98 D99 Q100 L101 F102 F103 I104 I105 G106 M109 I110 E111 Y112 L113 P114 K115 W116 Y117 K118 L119 D120 E121 L122

L125 G130 V131 LYS ARG PRO GLY PHE HIS V138 E139 T140 P141 Y142 P143 L144 L145 F146 A147 D148 V149 P150 E151 F152 E153 V154 S155 S156 T157 M158 I159 R160 E161 R162 F163 K164 S165 K166 K167 P168 T169 D170 Y171 L172 D175 K178 K179 V180 E183 N184 GLY LEU TYR GLU SER

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.31Å　　108.78Å　　177.56Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	15.00　–　3.20	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.279　,　0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9268	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

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	0.55	0/1588	0.83	3/2151 (0.1%)
1	B	0.68	4/1588 (0.3%)	0.99	12/2151 (0.6%)
1	C	0.52	0/1588	0.80	1/2151 (0.0%)
1	D	0.57	0/1588	0.81	2/2151 (0.1%)
1	E	0.38	0/1497	0.69	2/2024 (0.1%)
1	F	0.45	0/1416	0.98	8/1914 (0.4%)
All	All	0.53	4/9265 (0.0%)	0.86	28/12542 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	46	GLN	CB-CG	-7.89	1.31	1.52
1	B	45	LYS	C-O	7.04	1.36	1.23
1	B	46	GLN	C-O	5.13	1.33	1.23
1	B	45	LYS	CA-CB	-5.04	1.42	1.53

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	149	VAL	C-N-CD	-17.77	81.50	120.60
1	F	113	LEU	C-N-CD	-11.90	94.42	120.60
1	B	49	ASP	CB-CG-OD2	-11.83	107.65	118.30
1	F	81	GLY	N-CA-C	-9.92	88.31	113.10
1	B	55	HIS	N-CA-C	-8.17	88.94	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1542	0	1523	135	0
1	B	1542	0	1523	155	0
1	C	1542	0	1523	123	0
1	D	1542	0	1523	120	0
1	E	1456	0	1448	137	0
1	F	1380	0	1372	158	0
2	A	44	0	25	8	0
2	B	44	0	25	4	0
2	C	44	0	25	4	0
2	D	44	0	25	8	0
2	E	44	0	25	9	0
2	F	44	0	25	5	0
All	All	9268	0	9062	802	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 44.

The worst 5 of 802 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:F:149:VAL:CG1	1:F:150:PRO:HD3	1.68	1.23
1:B:10:THR:HG22	1:B:39:ASN:HD22	0.99	1.16
1:B:10:THR:HG22	1:B:39:ASN:ND2	1.68	1.08
1:F:113:LEU:HB3	1:F:114:PRO:HD2	1.32	1.08
1:F:149:VAL:HG12	1:F:150:PRO:CD	1.82	1.08

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	184/194 (95%)	139 (76%)	31 (17%)	14 (8%)	1	7
1	B	184/194 (95%)	145 (79%)	18 (10%)	21 (11%)	0	2
1	C	184/194 (95%)	151 (82%)	19 (10%)	14 (8%)	1	7
1	D	184/194 (95%)	144 (78%)	27 (15%)	13 (7%)	1	8
1	E	172/194 (89%)	142 (83%)	21 (12%)	9 (5%)	2	15
1	F	161/194 (83%)	111 (69%)	24 (15%)	26 (16%)	0	0
All	All	1069/1164 (92%)	832 (78%)	140 (13%)	97 (9%)	1	3

5 of 97 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	51	THR
1	A	52	ASP
1	A	79	ARG
1	A	80	GLU

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	171/177 (97%)	149 (87%)	22 (13%)	4	19
1	B	171/177 (97%)	149 (87%)	22 (13%)	4	19
1	C	171/177 (97%)	148 (86%)	23 (14%)	4	18
1	D	171/177 (97%)	147 (86%)	24 (14%)	3	16
1	E	161/177 (91%)	143 (89%)	18 (11%)	6	25
1	F	154/177 (87%)	127 (82%)	27 (18%)	2	9
All	All	999/1062 (94%)	863 (86%)	136 (14%)	3	17

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	60	LEU
1	F	77	MET
1	F	162	ARG
1	C	46	GLN
1	C	44	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	67	ASN
1	E	184	ASN
1	F	55	HIS
1	B	184	ASN
1	B	94	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

6 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	501	-	42,48,48	1.41	5 (11%)	50,73,73	1.26	5 (10%)
2	DND	E	201	-	42,48,48	1.41	5 (11%)	50,73,73	1.39	8 (16%)
2	DND	C	401	-	42,48,48	1.43	6 (14%)	50,73,73	1.38	7 (14%)
2	DND	A	601	-	42,48,48	1.39	5 (11%)	50,73,73	1.28	7 (14%)
2	DND	F	190	-	42,48,48	1.37	3 (7%)	50,73,73	1.43	7 (14%)
2	DND	D	301	-	42,48,48	1.38	6 (14%)	50,73,73	1.37	7 (14%)

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	501	-	3/3/11/11	9/26/62/62	0/5/5/5
2	DND	E	201	-	3/3/11/11	10/26/62/62	0/5/5/5
2	DND	C	401	-	3/3/11/11	8/26/62/62	0/5/5/5
2	DND	A	601	-	3/3/11/11	10/26/62/62	0/5/5/5
2	DND	F	190	-	3/3/11/11	12/26/62/62	0/5/5/5
2	DND	D	301	-	3/3/11/11	9/26/62/62	0/5/5/5

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	DND	O7N-C7N	4.74	1.36	1.22
2	B	501	DND	O7N-C7N	4.64	1.36	1.22
2	A	601	DND	O7N-C7N	4.51	1.36	1.22
2	D	301	DND	O7N-C7N	4.50	1.36	1.22
2	C	401	DND	O7N-C7N	4.47	1.35	1.22

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	DND	C6N-N1N-C2N	-5.57	116.89	121.97
2	E	201	DND	C6N-N1N-C2N	-5.46	117.00	121.97
2	D	301	DND	C6N-N1N-C2N	-5.08	117.34	121.97
2	F	190	DND	C6N-N1N-C2N	-5.03	117.39	121.97
2	A	601	DND	C6N-N1N-C2N	-4.91	117.50	121.97

5 of 18 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	DND	C3B
2	A	601	DND	C2B
2	A	601	DND	C1B
2	B	501	DND	C3B
2	B	501	DND	C2B

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	DND	C5D-O5D-PN-O12
2	A	601	DND	C5D-O5D-PN-O3P
2	A	601	DND	C5B-O5B-PA-O3P
2	A	601	DND	C5B-O5B-PA-O13
2	A	601	DND	C5B-O5B-PA-O14

There are no ring outliers.

6 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	DND	4	0
2	E	201	DND	9	0
2	C	401	DND	4	0
2	A	601	DND	8	0
2	F	190	DND	5	0
2	D	301	DND	8	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 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 DND B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand DND E 201

Bond lengths

Bond angles

Torsions

Rings

Ligand DND C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand DND A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand DND F 190

Bond lengths

Bond angles

Torsions

Rings

Ligand DND D 301

Bond lengths

Bond angles

Torsions

Rings
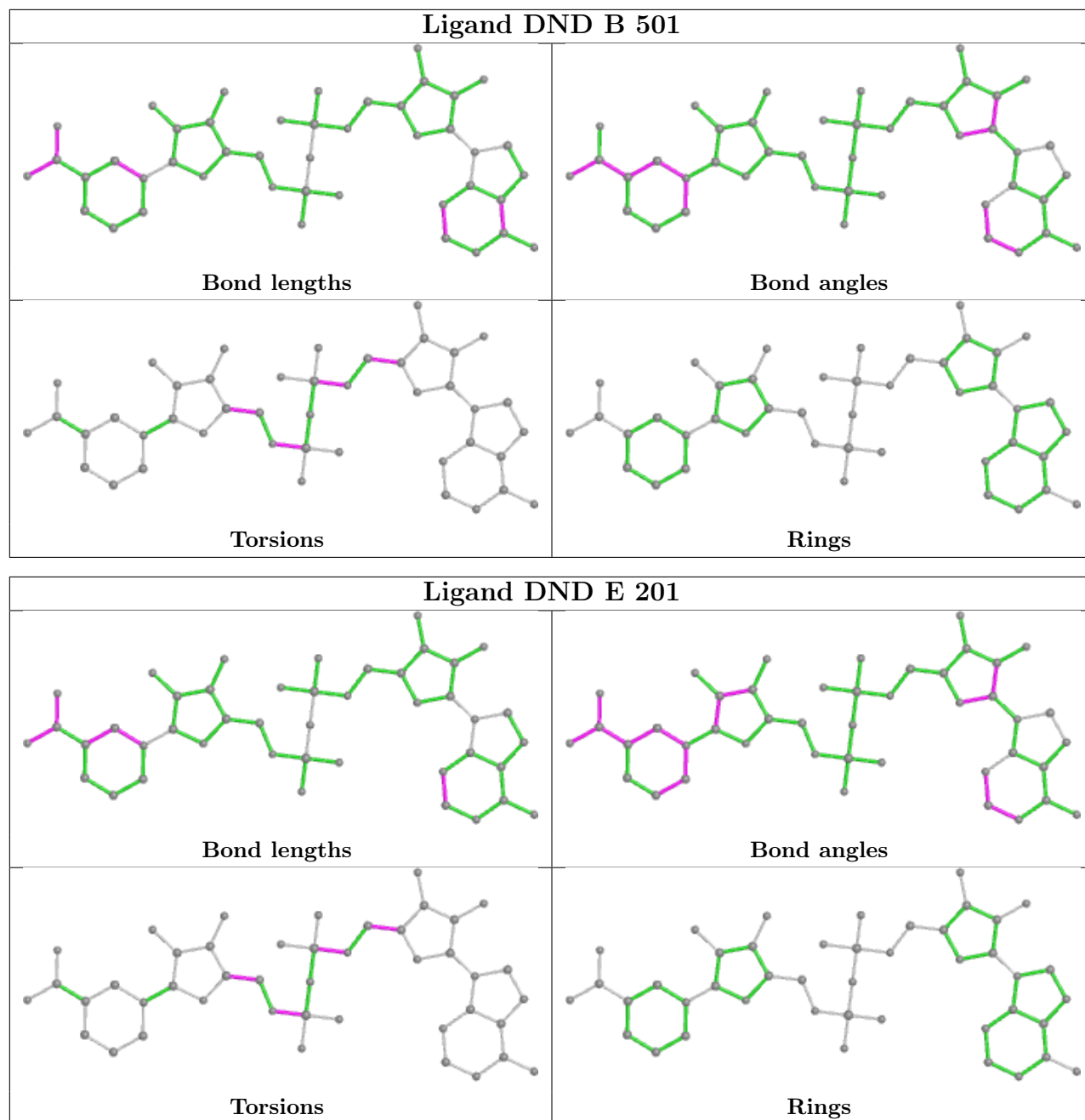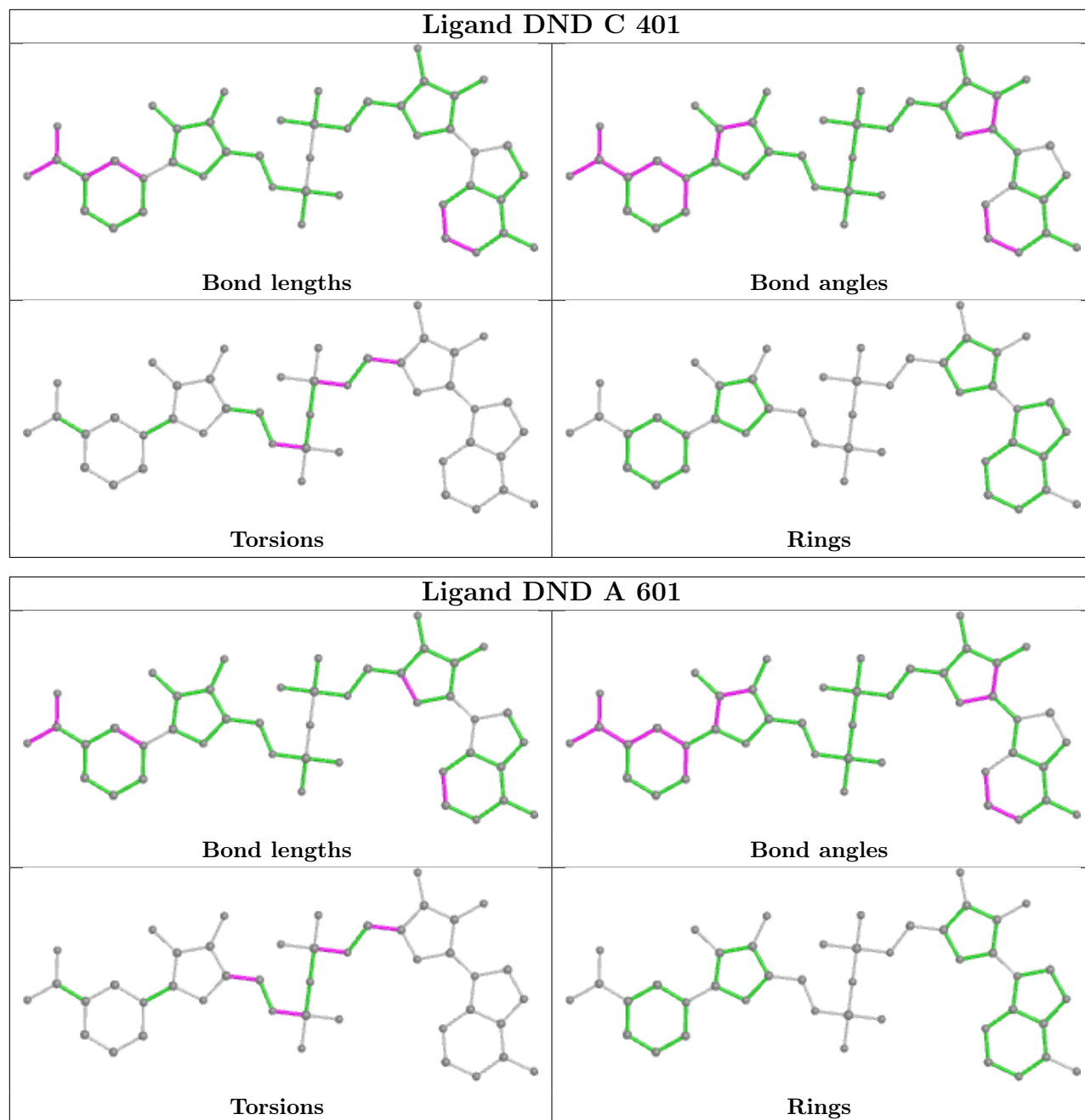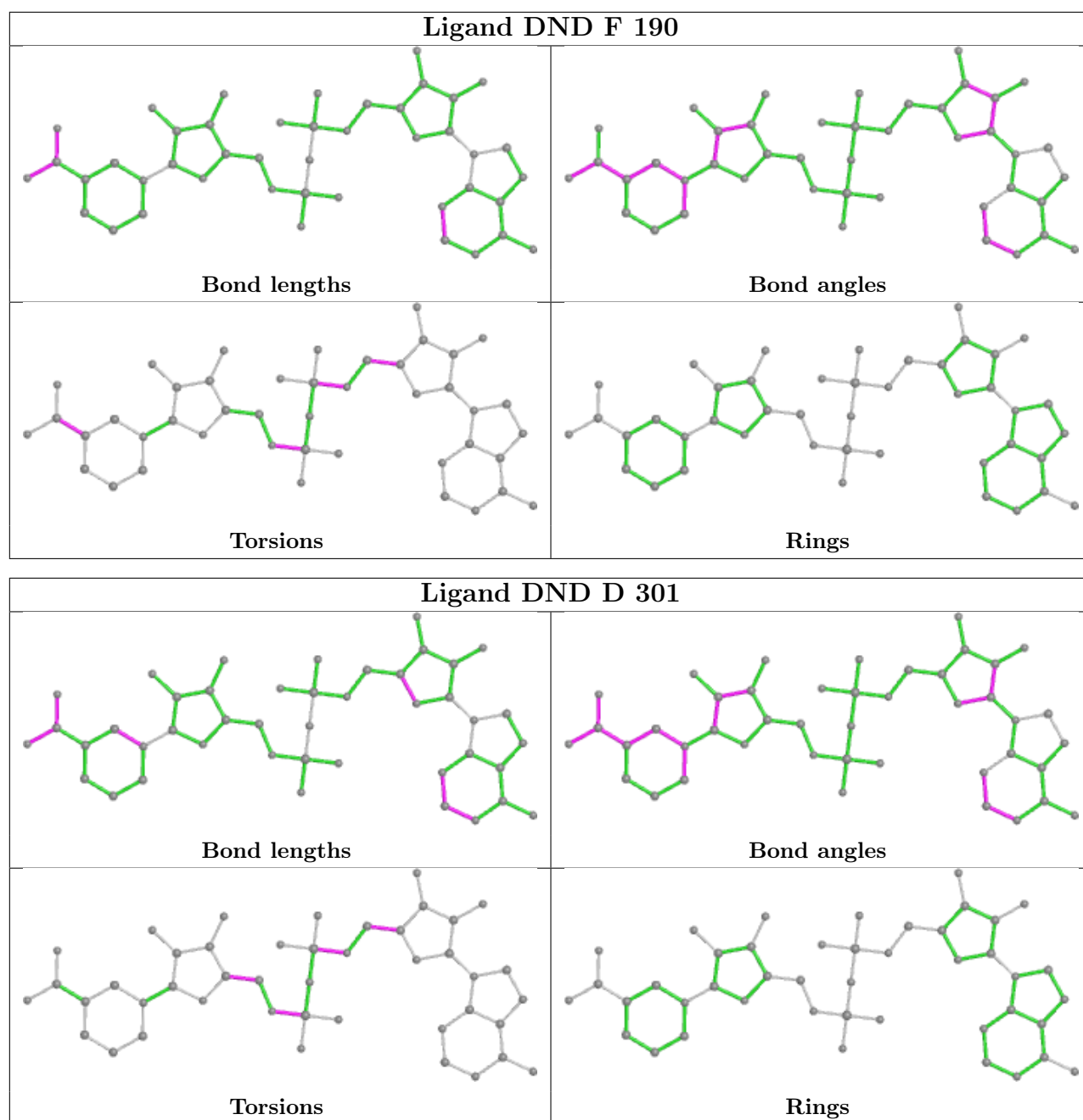
5.7 Other polymers ⓘ

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 ⓘ

6.1   Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3   Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4   Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5   Other polymers ⓘ

EDS was not executed - this section is therefore empty.