



## Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2023 – 03:25 PM EDT

PDB ID : 4OYR  
Title : Competition of the small inhibitor PT91 with large fatty acyl substrate of the Mycobacterium tuberculosis enoyl-ACP reductase InhA by induced substrate-binding loop refolding  
Authors : Li, H.J.; Pan, P.; Lai, C.T.; Liu, N.; Garcia-Diaz, M.; Simmerling, C.; Tonge, P.J.  
Deposited on : 2014-02-13  
Resolution : 2.30 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](mailto: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>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

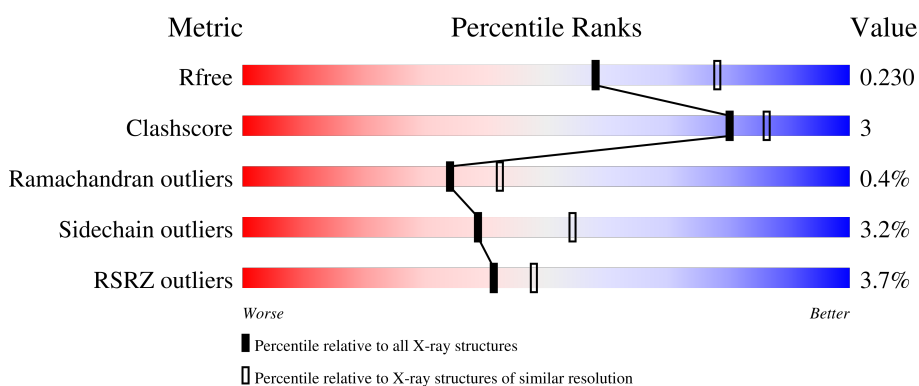
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	289	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2%      83%      10%      8%</p>
1	B	289	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">%      85%      7%      8%</p>
1	C	289	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 86%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">6%      86%      7%      7%</p>
1	D	289	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3%      82%      5% •      12%</p>

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7944 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
			Total	C	N	O	S			
1	A	267	Total 1967	C 1258	N 334	O 365	S 10	0	3	0
1	B	267	Total 1942	C 1234	N 339	O 359	S 10	0	0	0
1	C	268	Total 1932	C 1232	N 339	O 350	S 11	0	6	0
1	D	254	Total 1738	C 1111	N 307	O 309	S 11	0	2	3

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P0A5Y6
A	-18	GLY	-	expression tag	UNP P0A5Y6
A	-17	SER	-	expression tag	UNP P0A5Y6
A	-16	SER	-	expression tag	UNP P0A5Y6
A	-15	HIS	-	expression tag	UNP P0A5Y6
A	-14	HIS	-	expression tag	UNP P0A5Y6
A	-13	HIS	-	expression tag	UNP P0A5Y6
A	-12	HIS	-	expression tag	UNP P0A5Y6
A	-11	HIS	-	expression tag	UNP P0A5Y6
A	-10	HIS	-	expression tag	UNP P0A5Y6
A	-9	SER	-	expression tag	UNP P0A5Y6
A	-8	SER	-	expression tag	UNP P0A5Y6
A	-7	GLY	-	expression tag	UNP P0A5Y6
A	-6	LEU	-	expression tag	UNP P0A5Y6
A	-5	VAL	-	expression tag	UNP P0A5Y6
A	-4	PRO	-	expression tag	UNP P0A5Y6
A	-3	ARG	-	expression tag	UNP P0A5Y6
A	-2	GLY	-	expression tag	UNP P0A5Y6
A	-1	SER	-	expression tag	UNP P0A5Y6
A	0	HIS	-	expression tag	UNP P0A5Y6
B	-19	MET	-	expression tag	UNP P0A5Y6

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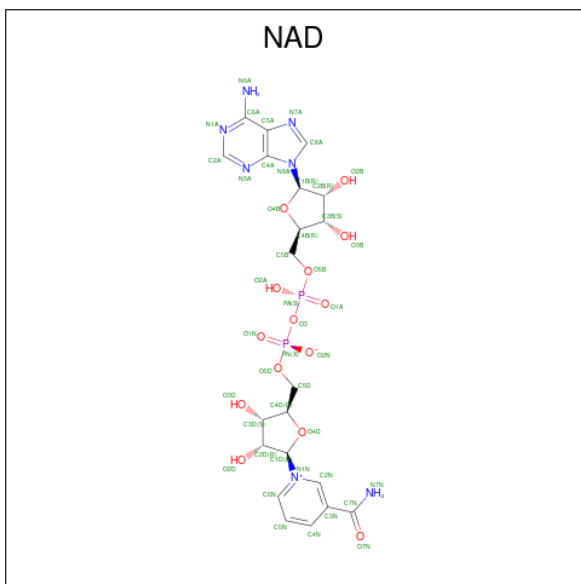
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P0A5Y6
B	-17	SER	-	expression tag	UNP P0A5Y6
B	-16	SER	-	expression tag	UNP P0A5Y6
B	-15	HIS	-	expression tag	UNP P0A5Y6
B	-14	HIS	-	expression tag	UNP P0A5Y6
B	-13	HIS	-	expression tag	UNP P0A5Y6
B	-12	HIS	-	expression tag	UNP P0A5Y6
B	-11	HIS	-	expression tag	UNP P0A5Y6
B	-10	HIS	-	expression tag	UNP P0A5Y6
B	-9	SER	-	expression tag	UNP P0A5Y6
B	-8	SER	-	expression tag	UNP P0A5Y6
B	-7	GLY	-	expression tag	UNP P0A5Y6
B	-6	LEU	-	expression tag	UNP P0A5Y6
B	-5	VAL	-	expression tag	UNP P0A5Y6
B	-4	PRO	-	expression tag	UNP P0A5Y6
B	-3	ARG	-	expression tag	UNP P0A5Y6
B	-2	GLY	-	expression tag	UNP P0A5Y6
B	-1	SER	-	expression tag	UNP P0A5Y6
B	0	HIS	-	expression tag	UNP P0A5Y6
C	-19	MET	-	expression tag	UNP P0A5Y6
C	-18	GLY	-	expression tag	UNP P0A5Y6
C	-17	SER	-	expression tag	UNP P0A5Y6
C	-16	SER	-	expression tag	UNP P0A5Y6
C	-15	HIS	-	expression tag	UNP P0A5Y6
C	-14	HIS	-	expression tag	UNP P0A5Y6
C	-13	HIS	-	expression tag	UNP P0A5Y6
C	-12	HIS	-	expression tag	UNP P0A5Y6
C	-11	HIS	-	expression tag	UNP P0A5Y6
C	-10	HIS	-	expression tag	UNP P0A5Y6
C	-9	SER	-	expression tag	UNP P0A5Y6
C	-8	SER	-	expression tag	UNP P0A5Y6
C	-7	GLY	-	expression tag	UNP P0A5Y6
C	-6	LEU	-	expression tag	UNP P0A5Y6
C	-5	VAL	-	expression tag	UNP P0A5Y6
C	-4	PRO	-	expression tag	UNP P0A5Y6
C	-3	ARG	-	expression tag	UNP P0A5Y6
C	-2	GLY	-	expression tag	UNP P0A5Y6
C	-1	SER	-	expression tag	UNP P0A5Y6
C	0	HIS	-	expression tag	UNP P0A5Y6
D	-19	MET	-	expression tag	UNP P0A5Y6
D	-18	GLY	-	expression tag	UNP P0A5Y6
D	-17	SER	-	expression tag	UNP P0A5Y6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP P0A5Y6
D	-15	HIS	-	expression tag	UNP P0A5Y6
D	-14	HIS	-	expression tag	UNP P0A5Y6
D	-13	HIS	-	expression tag	UNP P0A5Y6
D	-12	HIS	-	expression tag	UNP P0A5Y6
D	-11	HIS	-	expression tag	UNP P0A5Y6
D	-10	HIS	-	expression tag	UNP P0A5Y6
D	-9	SER	-	expression tag	UNP P0A5Y6
D	-8	SER	-	expression tag	UNP P0A5Y6
D	-7	GLY	-	expression tag	UNP P0A5Y6
D	-6	LEU	-	expression tag	UNP P0A5Y6
D	-5	VAL	-	expression tag	UNP P0A5Y6
D	-4	PRO	-	expression tag	UNP P0A5Y6
D	-3	ARG	-	expression tag	UNP P0A5Y6
D	-2	GLY	-	expression tag	UNP P0A5Y6
D	-1	SER	-	expression tag	UNP P0A5Y6
D	0	HIS	-	expression tag	UNP P0A5Y6

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



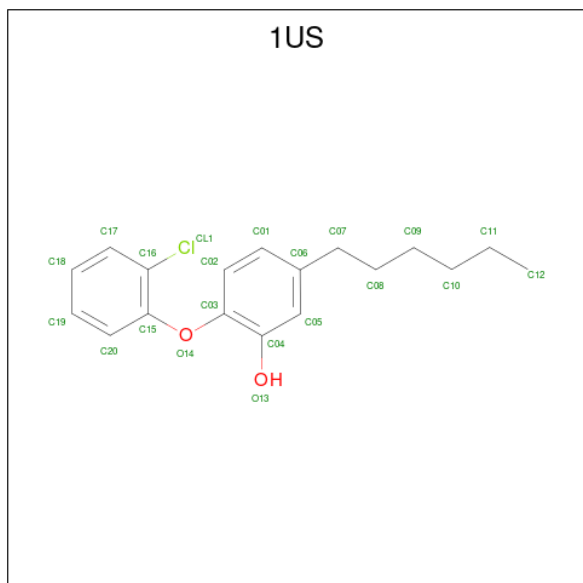
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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

- Molecule 3 is 2-(2-chloranylphenoxy)-5-hexyl-phenol (three-letter code: 1US) (formula:  $C_{18}H_{21}ClO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	O	0	0
			19	16	1	2		
3	B	1	Total	C	Cl	O	0	0
			20	17	1	2		
3	C	1	Total	C	Cl	O	0	0
			19	16	1	2		
3	D	1	Total	C	Cl	O	0	0
			20	17	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	31	Total	O	0	0
			31	31		
4	C	28	Total	O	0	0
			28	28		

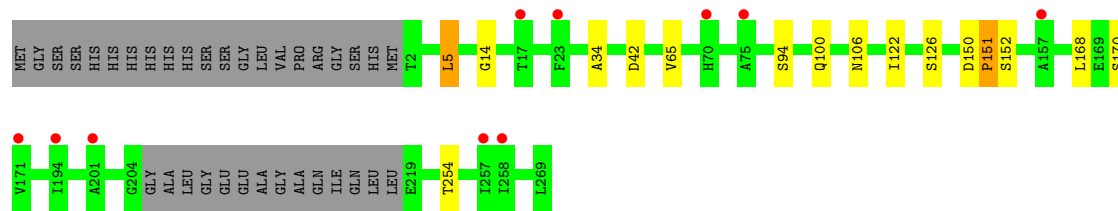
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	D	8	Total	O	0	0
			8	8		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.84Å 90.65Å 164.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.70 – 2.30 43.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.8 (43.70-2.30) 80.0 (43.70-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 2.29Å)	Xtrriage
Refinement program	PHENIX, CNS	Depositor
R, $R_{free}$	0.194 , 0.244 0.181 , 0.230	Depositor DCC
$R_{free}$ test set	2284 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.3	Xtrriage
Anisotropy	0.918	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1US, 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	0.38	0/2005	0.55	0/2727
1	B	0.37	0/1980	0.53	0/2691
1	C	0.36	0/1970	0.53	0/2668
1	D	0.29	0/1774	0.47	0/2396
All	All	0.35	0/7729	0.52	0/10482

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1967	0	1955	14	0
1	B	1942	0	1923	11	0
1	C	1932	0	1873	9	0
1	D	1738	0	1633	8	0
2	A	44	0	26	1	0
2	B	44	0	26	1	0
2	C	44	0	26	2	0
2	D	44	0	26	2	0
3	A	19	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	16	0	0
3	C	19	0	14	0	0
3	D	20	0	16	0	0
4	A	44	0	0	0	0
4	B	31	0	0	0	0
4	C	28	0	0	0	0
4	D	8	0	0	0	0
All	All	7944	0	7548	41	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 3.

All (41) 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:C:17:THR:HA	1:C:50:ILE:HD13	1.73	0.69
1:D:5:LEU:HB3	1:D:34:ALA:HB2	1.76	0.68
1:B:17:THR:HA	1:B:50:ILE:HD13	1.79	0.63
1:B:157:ALA:HB2	1:B:207:LEU:HD21	1.81	0.61
1:C:44:LEU:HD11	1:C:62:GLU:HB2	1.83	0.60
2:D:301:NAD:O1N	2:D:301:NAD:H2N	2.02	0.59
1:C:49:ARG:O	1:C:52:ASP:HB2	2.07	0.53
1:A:16:ILE:O	1:A:50:ILE:HD13	2.10	0.51
1:B:134:LEU:O	1:B:138:MET:HG3	2.11	0.50
2:C:301:NAD:H2N	2:C:301:NAD:O1N	2.10	0.50
1:A:157:ALA:HB2	1:A:207:LEU:HD21	1.94	0.49
1:B:20:SER:OG	2:B:301:NAD:O1A	2.27	0.48
1:C:47:ILE:O	1:C:51:THR:HG23	2.13	0.47
1:A:46[A]:LEU:O	1:A:50:ILE:HD12	2.15	0.46
1:A:121:HIS:HB2	1:C:113:TYR:CE2	2.50	0.46
1:A:10:ILE:HD13	1:A:246:LEU:HD13	1.99	0.45
1:C:65:VAL:HG22	2:C:301:NAD:N1A	2.32	0.45
1:A:193:PRO:O	1:A:232:MET:HG3	2.17	0.45
1:B:130:MET:HE3	1:B:130:MET:HB3	1.91	0.44
1:A:46[B]:LEU:O	1:A:50:ILE:HD12	2.17	0.44
1:B:245:LEU:HD21	1:B:258:ILE:HD13	2.00	0.44
1:C:145[A]:VAL:HA	1:C:187:ASN:O	2.18	0.43
1:A:110:ASP:OD1	1:C:132:LYS:NZ	2.52	0.43
1:C:134:LEU:O	1:C:138:MET:HG3	2.19	0.43
1:D:122:ILE:O	1:D:126:SER:OG	2.28	0.43
1:A:65:VAL:HG22	2:A:301:NAD:N1A	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LEU:HD11	1:B:258:ILE:HD13	2.00	0.42
1:D:150:ASP:OD1	1:D:152:SER:OG	2.34	0.42
1:D:65:VAL:HG22	2:D:301:NAD:N1A	2.34	0.42
1:D:14:GLY:HA3	1:D:94:SER:O	2.19	0.42
1:B:165:LYS:HD3	1:B:165:LYS:HA	1.69	0.42
1:A:199:MET:HE3	3:A:302:1US:H6	2.02	0.42
1:A:199:MET:CE	3:A:302:1US:H6	2.50	0.42
1:A:228:ILE:HG23	1:D:254:THR:HG21	2.01	0.42
1:B:126:SER:HA	1:B:129:SER:HB2	2.02	0.42
1:D:150:ASP:HA	1:D:151:PRO:HD3	1.86	0.41
1:D:100:GLN:O	1:D:106:ASN:ND2	2.53	0.41
1:A:39:THR:HA	1:A:61:LEU:O	2.21	0.41
1:B:39:THR:HA	1:B:61:LEU:O	2.20	0.41
1:B:46:LEU:HD23	1:B:46:LEU:HA	1.90	0.40
1:A:134:LEU:O	1:A:138:MET:HG3	2.21	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	268/289 (93%)	257 (96%)	9 (3%)	2 (1%)	22	26
1	B	265/289 (92%)	254 (96%)	11 (4%)	0	100	100
1	C	272/289 (94%)	261 (96%)	11 (4%)	0	100	100
1	D	250/289 (86%)	236 (94%)	12 (5%)	2 (1%)	19	23
All	All	1055/1156 (91%)	1008 (96%)	43 (4%)	4 (0%)	34	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	ASP
1	A	42	ASP
1	A	159	ASN
1	D	151	PRO

### 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	193/222 (87%)	183 (95%)	10 (5%)	23	32
1	B	190/222 (86%)	184 (97%)	6 (3%)	39	54
1	C	182/222 (82%)	172 (94%)	10 (6%)	21	30
1	D	155/222 (70%)	151 (97%)	4 (3%)	46	63
All	All	720/888 (81%)	690 (96%)	30 (4%)	39	42

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	44	LEU
1	A	71	LEU
1	A	74	LEU
1	A	162	THR
1	A	168[A]	LEU
1	A	168[B]	LEU
1	A	170	SER
1	A	197[A]	LEU
1	A	197[B]	LEU
1	B	5	LEU
1	B	130	MET
1	B	162	THR
1	B	168	LEU
1	B	247	SER
1	B	269	LEU
1	C	6	ASP
1	C	43[A]	ARG

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Mol	Chain	Res	Type
1	C	43[B]	ARG
1	C	71[A]	LEU
1	C	71[B]	LEU
1	C	145[A]	VAL
1	C	145[B]	VAL
1	C	168[A]	LEU
1	C	168[B]	LEU
1	C	170	SER
1	D	5	LEU
1	D	168[A]	LEU
1	D	168[B]	LEU
1	D	170	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

8 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	1US	B	302	-	21,21,22	0.78	1 (4%)	27,27,28	0.97	0
2	NAD	A	301	-	42,48,48	3.23	20 (47%)	50,73,73	1.53	7 (14%)
3	1US	D	302	-	21,21,22	0.91	1 (4%)	27,27,28	0.81	2 (7%)
2	NAD	D	301	-	42,48,48	3.18	21 (50%)	50,73,73	1.59	11 (22%)
3	1US	A	302	-	20,20,22	0.80	2 (10%)	26,26,28	0.90	1 (3%)
2	NAD	C	301	-	42,48,48	3.26	20 (47%)	50,73,73	1.53	7 (14%)
2	NAD	B	301	-	42,48,48	3.17	18 (42%)	50,73,73	1.57	9 (18%)
3	1US	C	302	-	20,20,22	0.92	1 (5%)	26,26,28	0.70	0

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
3	1US	B	302	-	-	2/9/9/10	0/2/2/2
2	NAD	A	301	-	-	7/26/62/62	0/5/5/5
3	1US	D	302	-	-	3/9/9/10	0/2/2/2
2	NAD	D	301	-	-	11/26/62/62	0/5/5/5
3	1US	A	302	-	-	1/8/8/10	0/2/2/2
2	NAD	C	301	-	-	10/26/62/62	0/5/5/5
2	NAD	B	301	-	-	7/26/62/62	0/5/5/5
3	1US	C	302	-	-	1/8/8/10	0/2/2/2

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAD	C2N-N1N	9.16	1.46	1.35
2	B	301	NAD	C2N-N1N	8.98	1.45	1.35
2	C	301	NAD	C2N-N1N	8.96	1.45	1.35
2	D	301	NAD	C2N-N1N	8.36	1.45	1.35
2	A	301	NAD	C7N-N7N	7.59	1.47	1.33
2	B	301	NAD	C7N-N7N	7.14	1.46	1.33
2	D	301	NAD	C7N-N7N	7.01	1.46	1.33
2	C	301	NAD	C7N-N7N	6.98	1.46	1.33
2	D	301	NAD	C4N-C3N	6.43	1.50	1.39
2	C	301	NAD	C4N-C3N	6.37	1.50	1.39
2	B	301	NAD	C4N-C3N	6.13	1.49	1.39
2	C	301	NAD	C2A-N3A	6.10	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NAD	C2A-N3A	6.03	1.41	1.32
2	A	301	NAD	C4N-C3N	5.81	1.49	1.39
2	C	301	NAD	C6N-N1N	5.81	1.49	1.35
2	B	301	NAD	C6N-N1N	5.69	1.49	1.35
2	A	301	NAD	C6N-N1N	5.61	1.49	1.35
2	B	301	NAD	C8A-N7A	5.59	1.44	1.34
2	A	301	NAD	C2A-N3A	5.56	1.41	1.32
2	B	301	NAD	C2A-N3A	5.48	1.40	1.32
2	D	301	NAD	C6N-N1N	5.43	1.48	1.35
2	C	301	NAD	C8A-N7A	5.17	1.43	1.34
2	D	301	NAD	C8A-N7A	5.16	1.43	1.34
2	A	301	NAD	C8A-N7A	4.97	1.43	1.34
2	D	301	NAD	C2A-N1A	4.82	1.42	1.33
2	A	301	NAD	C2N-C3N	4.69	1.46	1.39
2	C	301	NAD	C2A-N1A	4.66	1.42	1.33
2	C	301	NAD	C2N-C3N	4.58	1.46	1.39
2	B	301	NAD	C2A-N1A	4.57	1.42	1.33
2	D	301	NAD	PA-O1A	4.24	1.66	1.50
2	B	301	NAD	PA-O1A	4.22	1.65	1.50
2	A	301	NAD	PN-O1N	4.11	1.65	1.50
2	C	301	NAD	PA-O1A	4.11	1.65	1.50
2	A	301	NAD	PA-O1A	4.09	1.65	1.50
2	A	301	NAD	C2A-N1A	4.07	1.41	1.33
2	B	301	NAD	C2N-C3N	4.05	1.45	1.39
2	C	301	NAD	PN-O1N	3.91	1.64	1.50
2	D	301	NAD	PN-O1N	3.90	1.64	1.50
2	D	301	NAD	C2N-C3N	3.84	1.45	1.39
2	C	301	NAD	C6N-C5N	3.56	1.46	1.38
2	B	301	NAD	C6A-N6A	3.45	1.46	1.34
2	D	301	NAD	C6A-N6A	3.44	1.46	1.34
2	A	301	NAD	C6A-N6A	3.44	1.46	1.34
2	A	301	NAD	C6N-C5N	3.44	1.46	1.38
2	C	301	NAD	C6A-N6A	3.43	1.46	1.34
2	D	301	NAD	C6N-C5N	3.31	1.46	1.38
2	C	301	NAD	C3B-C4B	3.30	1.61	1.53
2	B	301	NAD	PN-O1N	3.28	1.62	1.50
2	B	301	NAD	C6N-C5N	3.19	1.45	1.38
2	C	301	NAD	O7N-C7N	-3.18	1.18	1.24
2	A	301	NAD	C3B-C4B	3.11	1.60	1.53
2	C	301	NAD	C5N-C4N	3.07	1.45	1.38
2	D	301	NAD	C3B-C4B	3.06	1.60	1.53
2	D	301	NAD	O7N-C7N	-3.05	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAD	C3N-C7N	2.96	1.55	1.50
2	B	301	NAD	C2B-C1B	-2.91	1.49	1.53
2	A	301	NAD	C5N-C4N	2.89	1.45	1.38
2	D	301	NAD	C5N-C4N	2.85	1.44	1.38
2	B	301	NAD	C3B-C4B	2.83	1.60	1.53
2	D	301	NAD	C2B-C1B	-2.80	1.49	1.53
2	D	301	NAD	C3N-C7N	2.74	1.54	1.50
2	A	301	NAD	O7N-C7N	-2.62	1.19	1.24
2	A	301	NAD	C2B-C1B	-2.56	1.49	1.53
2	C	301	NAD	C2B-C1B	-2.50	1.50	1.53
2	B	301	NAD	O7N-C7N	-2.46	1.19	1.24
2	A	301	NAD	C2D-C1D	-2.43	1.50	1.53
2	B	301	NAD	C5N-C4N	2.42	1.44	1.38
2	B	301	NAD	C3N-C7N	2.36	1.54	1.50
2	C	301	NAD	C2D-C1D	-2.31	1.50	1.53
2	C	301	NAD	C3N-C7N	2.30	1.54	1.50
2	A	301	NAD	C3D-C4D	2.28	1.58	1.53
2	B	301	NAD	C3D-C4D	2.25	1.58	1.53
2	C	301	NAD	C3D-C4D	2.19	1.58	1.53
3	D	302	1US	C16-CL1	2.19	1.78	1.73
3	C	302	1US	C16-CL1	2.17	1.78	1.73
3	B	302	1US	C16-CL1	2.17	1.78	1.73
2	C	301	NAD	O4B-C4B	2.16	1.49	1.45
2	D	301	NAD	C3D-C4D	2.11	1.58	1.53
2	D	301	NAD	PA-O5B	2.08	1.67	1.59
3	A	302	1US	O13-C04	2.06	1.40	1.36
2	D	301	NAD	O4B-C4B	2.04	1.49	1.45
2	A	301	NAD	PN-O5D	2.04	1.67	1.59
3	A	302	1US	C16-CL1	2.02	1.78	1.73
2	D	301	NAD	PN-O5D	2.01	1.67	1.59

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAD	N3A-C2A-N1A	-5.78	119.64	128.68
2	A	301	NAD	N3A-C2A-N1A	-5.73	119.73	128.68
2	B	301	NAD	N3A-C2A-N1A	-5.68	119.80	128.68
2	D	301	NAD	N3A-C2A-N1A	-5.47	120.13	128.68
2	D	301	NAD	PN-O3-PA	-4.46	117.51	132.83
2	C	301	NAD	PN-O3-PA	-3.73	120.04	132.83
2	A	301	NAD	PN-O3-PA	-3.36	121.29	132.83
2	B	301	NAD	PN-O3-PA	-3.24	121.71	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAD	C3D-C2D-C1D	-3.19	96.18	100.98
2	A	301	NAD	C3D-C2D-C1D	-2.98	96.50	100.98
2	C	301	NAD	C3D-C2D-C1D	-2.74	96.86	100.98
2	B	301	NAD	O4B-C4B-C5B	2.55	117.76	109.37
3	D	302	1US	O14-C03-C04	2.47	120.84	116.22
2	D	301	NAD	O4D-C4D-C5D	2.47	117.49	109.37
3	A	302	1US	O14-C03-C04	2.39	120.70	116.22
2	D	301	NAD	O3B-C3B-C4B	2.38	117.94	111.05
2	A	301	NAD	O2D-C2D-C1D	2.36	119.56	110.85
2	B	301	NAD	O3B-C3B-C2B	2.34	119.40	111.82
2	D	301	NAD	O2D-C2D-C1D	2.33	119.47	110.85
2	A	301	NAD	C6N-N1N-C2N	-2.33	119.85	121.97
2	D	301	NAD	O3B-C3B-C2B	2.29	119.22	111.82
2	B	301	NAD	O3D-C3D-C4D	2.27	117.60	111.05
2	A	301	NAD	O4B-C4B-C5B	2.26	116.81	109.37
2	B	301	NAD	C2N-C3N-C4N	2.25	120.81	118.26
2	D	301	NAD	O3D-C3D-C4D	2.17	117.31	111.05
2	D	301	NAD	C3D-C2D-C1D	-2.16	97.72	100.98
2	A	301	NAD	O4B-C1B-C2B	-2.16	103.77	106.93
2	C	301	NAD	C2N-C3N-C4N	2.16	120.70	118.26
2	B	301	NAD	C3B-C2B-C1B	-2.15	97.74	100.98
2	C	301	NAD	C3N-C7N-N7N	2.14	120.32	117.75
2	D	301	NAD	O2B-C2B-C1B	2.12	118.68	110.85
2	C	301	NAD	O3B-C3B-C4B	2.11	117.16	111.05
2	C	301	NAD	C6N-N1N-C2N	-2.08	120.08	121.97
2	D	301	NAD	O5B-C5B-C4B	2.07	116.11	108.99
3	D	302	1US	C03-O14-C15	-2.01	113.26	118.04
2	D	301	NAD	O2D-C2D-C3D	2.00	118.30	111.82
2	B	301	NAD	C5B-C4B-C3B	-2.00	107.68	115.18

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAD	C5D-O5D-PN-O1N
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	301	NAD	C5D-O5D-PN-O1N
2	B	301	NAD	C5D-O5D-PN-O2N
2	B	301	NAD	O4D-C1D-N1N-C2N
2	B	301	NAD	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
2	C	301	NAD	C5D-O5D-PN-O1N
2	C	301	NAD	C5D-O5D-PN-O2N
2	C	301	NAD	O4D-C1D-N1N-C2N
2	C	301	NAD	O4D-C1D-N1N-C6N
2	D	301	NAD	C5B-O5B-PA-O1A
2	D	301	NAD	C5B-O5B-PA-O3
2	D	301	NAD	PN-O3-PA-O5B
2	D	301	NAD	PA-O3-PN-O5D
2	D	301	NAD	C5D-O5D-PN-O3
2	D	301	NAD	O4D-C1D-N1N-C2N
2	D	301	NAD	O4B-C4B-C5B-O5B
2	D	301	NAD	C3B-C4B-C5B-O5B
3	C	302	1US	C06-C07-C08-C09
3	A	302	1US	C06-C07-C08-C09
3	D	302	1US	C06-C07-C08-C09
3	D	302	1US	C08-C09-C10-C11
3	B	302	1US	C06-C07-C08-C09
2	C	301	NAD	O4B-C4B-C5B-O5B
2	A	301	NAD	PN-O3-PA-O5B
2	B	301	NAD	PN-O3-PA-O5B
2	C	301	NAD	PN-O3-PA-O5B
2	C	301	NAD	C5B-O5B-PA-O3
3	D	302	1US	C07-C08-C09-C10
2	C	301	NAD	C5B-O5B-PA-O1A
2	D	301	NAD	C5D-O5D-PN-O1N
3	B	302	1US	C07-C08-C09-C10
2	D	301	NAD	C4B-C5B-O5B-PA
2	B	301	NAD	O4B-C4B-C5B-O5B
2	D	301	NAD	C4D-C5D-O5D-PN
2	A	301	NAD	C5D-O5D-PN-O3
2	B	301	NAD	C5D-O5D-PN-O3
2	C	301	NAD	C5D-O5D-PN-O3
2	C	301	NAD	C3B-C4B-C5B-O5B
2	A	301	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

5 monomers are involved in 8 short contacts:

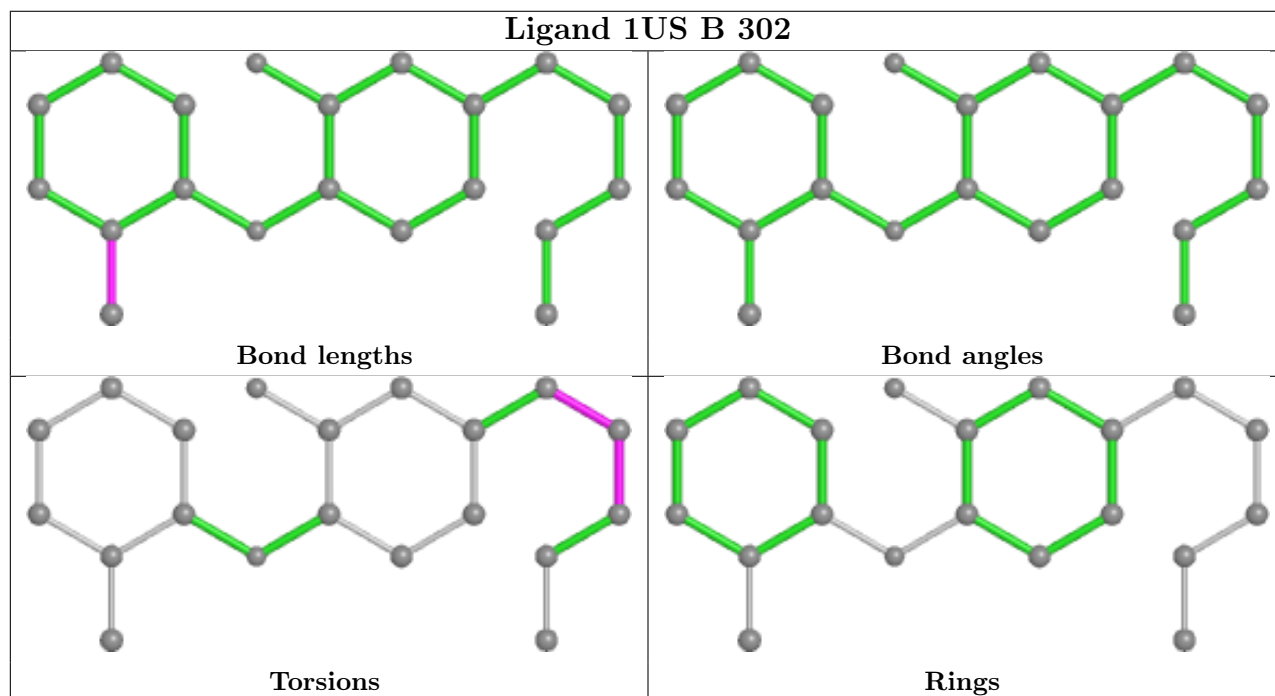
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAD	1	0
2	D	301	NAD	2	0
3	A	302	1US	2	0

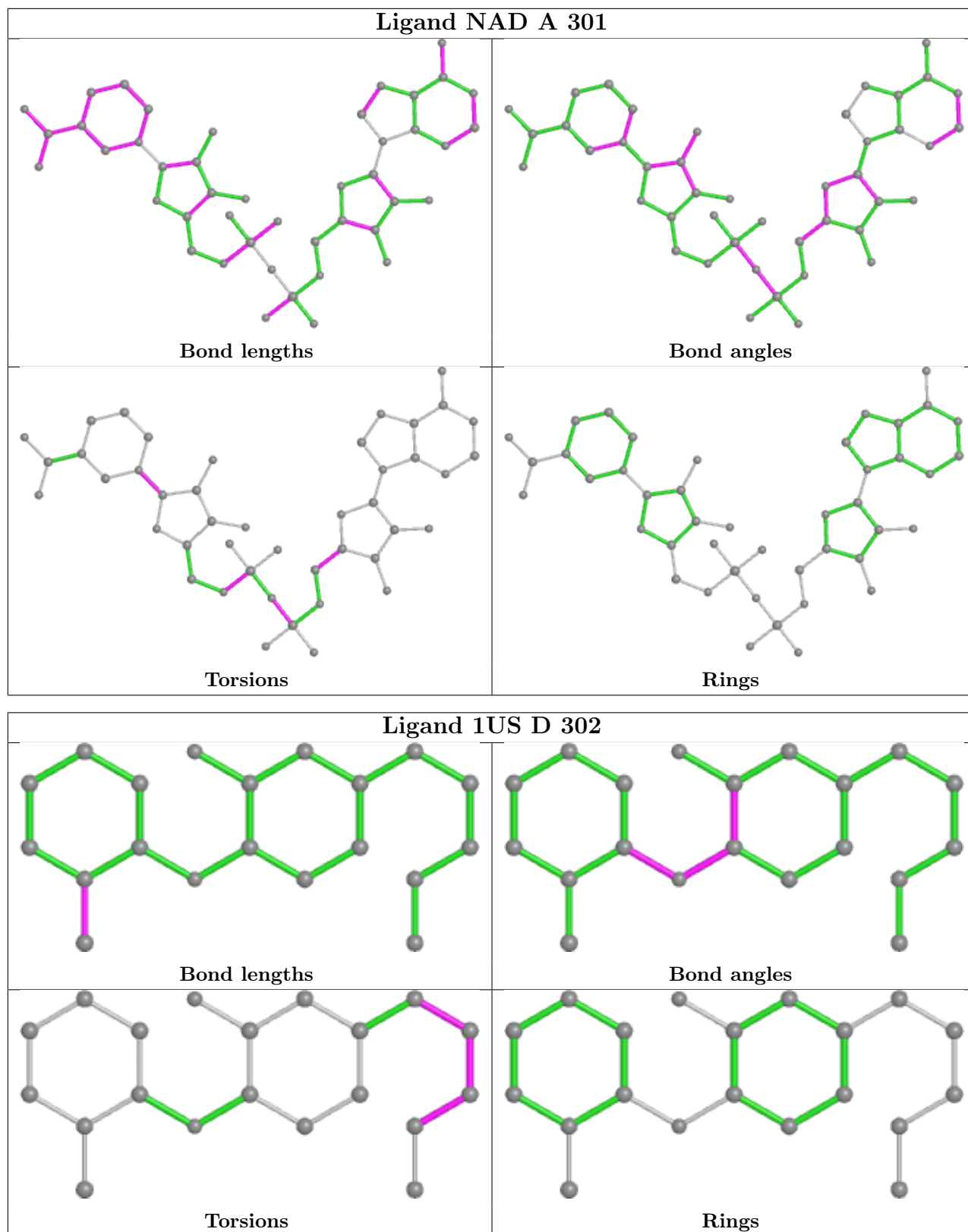
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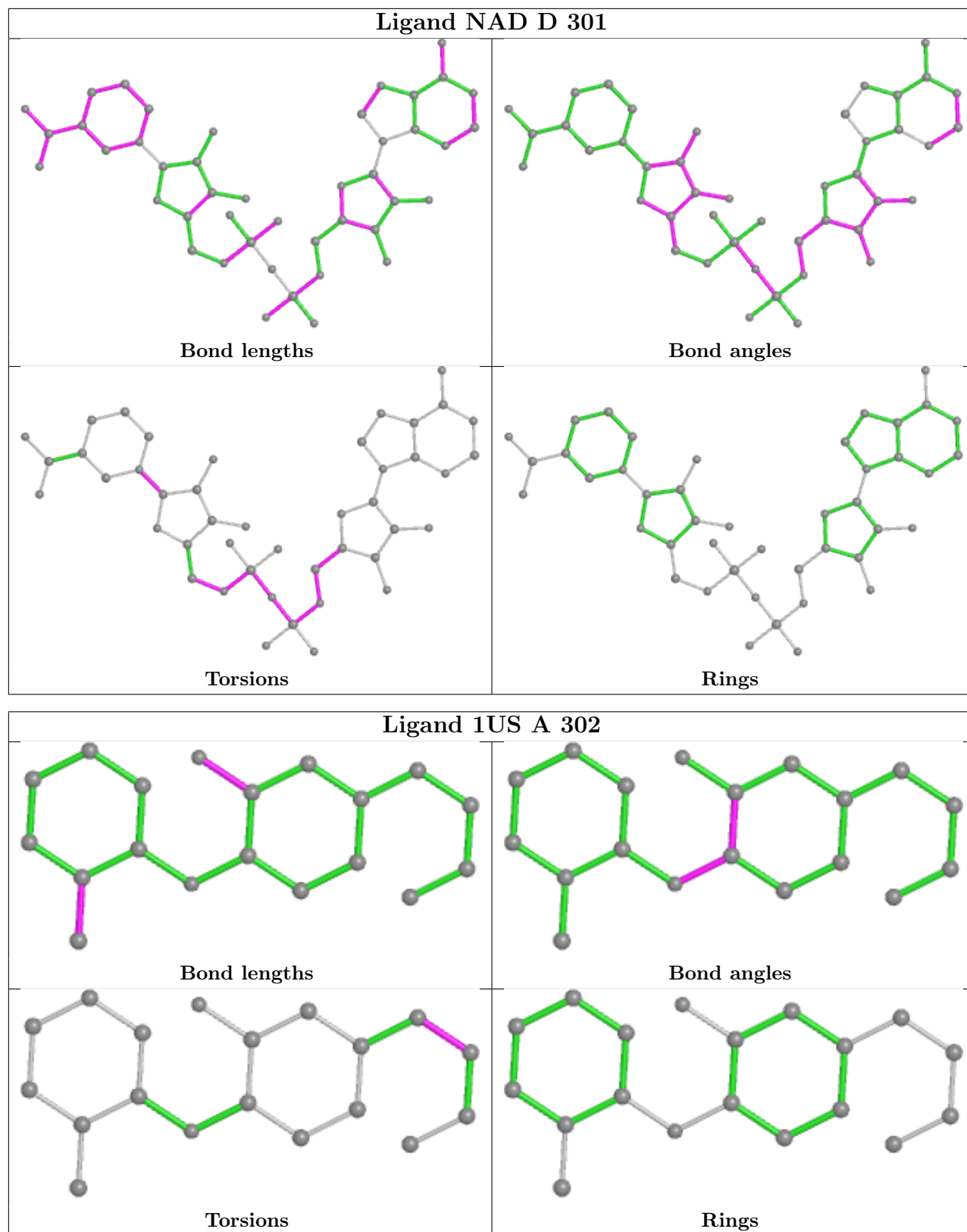
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	NAD	2	0
2	B	301	NAD	1	0

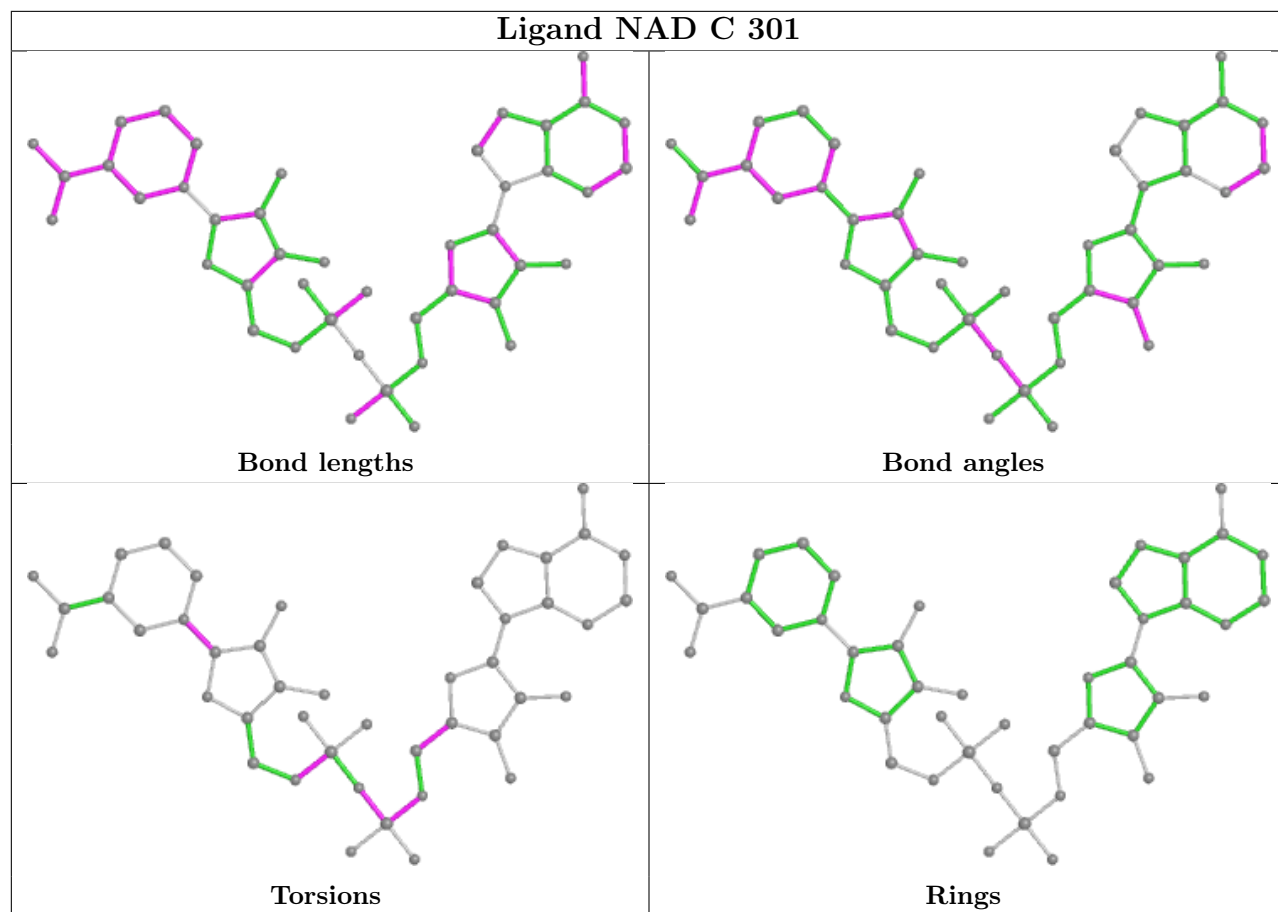
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

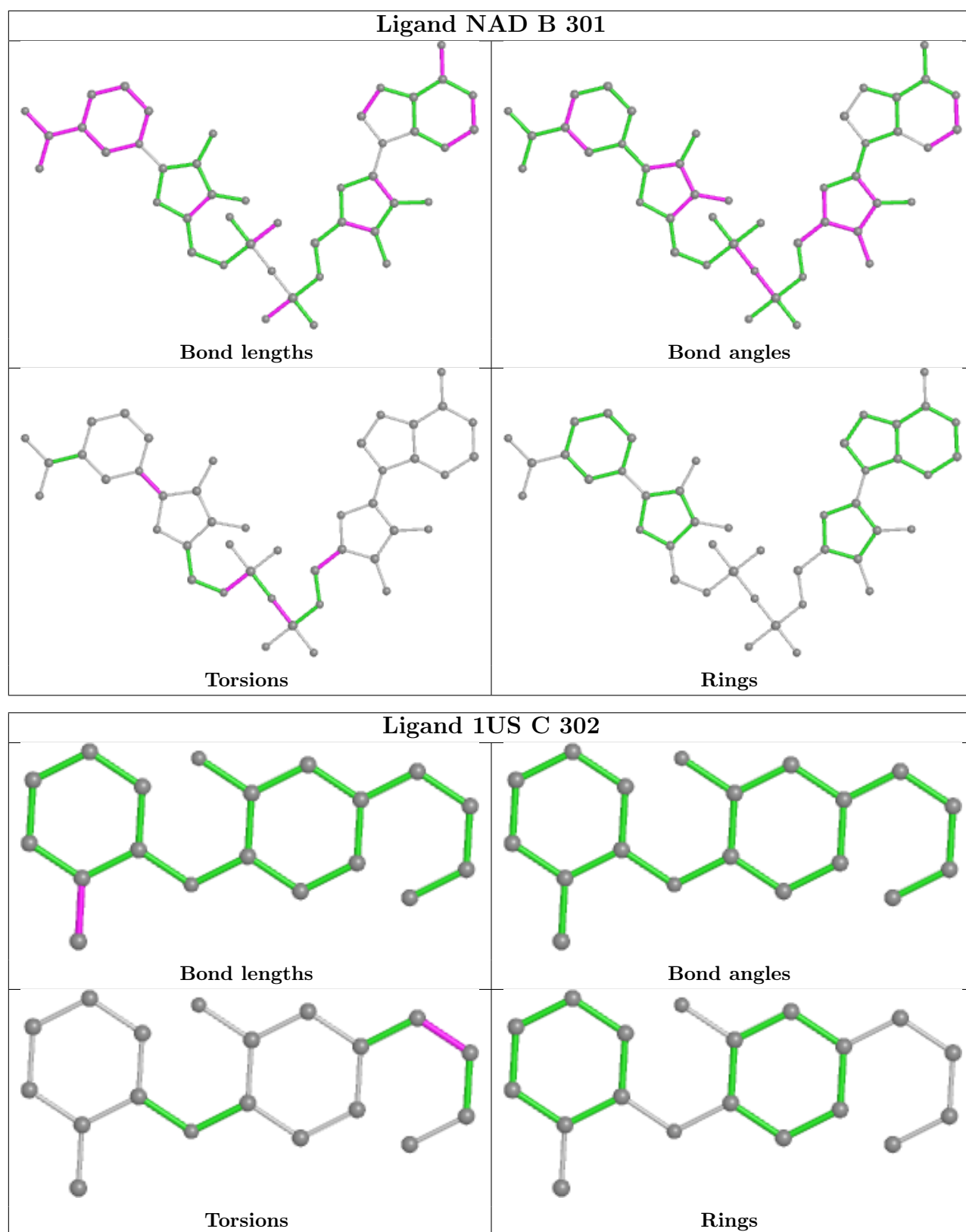












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	267/289 (92%)	-0.14	7 (2%) 56 63	23, 38, 53, 64	0
1	B	267/289 (92%)	-0.13	4 (1%) 73 79	26, 43, 58, 75	0
1	C	268/289 (92%)	0.20	18 (6%) 17 23	26, 44, 74, 93	0
1	D	254/289 (87%)	0.22	10 (3%) 39 46	31, 57, 79, 91	0
All	All	1056/1156 (91%)	0.04	39 (3%) 41 48	23, 44, 72, 93	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	213	ALA	6.1
1	C	211	ALA	5.0
1	C	212	GLY	4.5
1	C	208	GLY	4.0
1	C	202	ILE	3.6
1	C	201	ALA	3.4
1	C	203	VAL	3.3
1	C	205	GLY	3.1
1	C	210	GLU	3.0
1	C	209	GLU	2.9
1	C	207	LEU	2.9
1	D	201	ALA	2.8
1	A	257	ILE	2.8
1	C	259	TYR	2.8
1	C	215	ILE	2.7
1	A	259	TYR	2.6
1	A	266	THR	2.5
1	C	204	GLY	2.4
1	D	257	ILE	2.4
1	C	188	LEU	2.3
1	B	257	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	157	ALA	2.3
1	D	70	HIS	2.3
1	A	152	SER	2.3
1	C	206	ALA	2.2
1	D	23	PHE	2.2
1	B	152	SER	2.2
1	B	258	ILE	2.2
1	B	259	TYR	2.2
1	C	257	ILE	2.2
1	A	213	ALA	2.2
1	D	258	ILE	2.1
1	A	265	HIS	2.1
1	C	214	GLN	2.1
1	D	75	ALA	2.1
1	D	17	THR	2.1
1	D	171	VAL	2.0
1	A	188	LEU	2.0
1	D	194	ILE	2.0

## 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 monosaccharides 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, 95<sup>th</sup> 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.

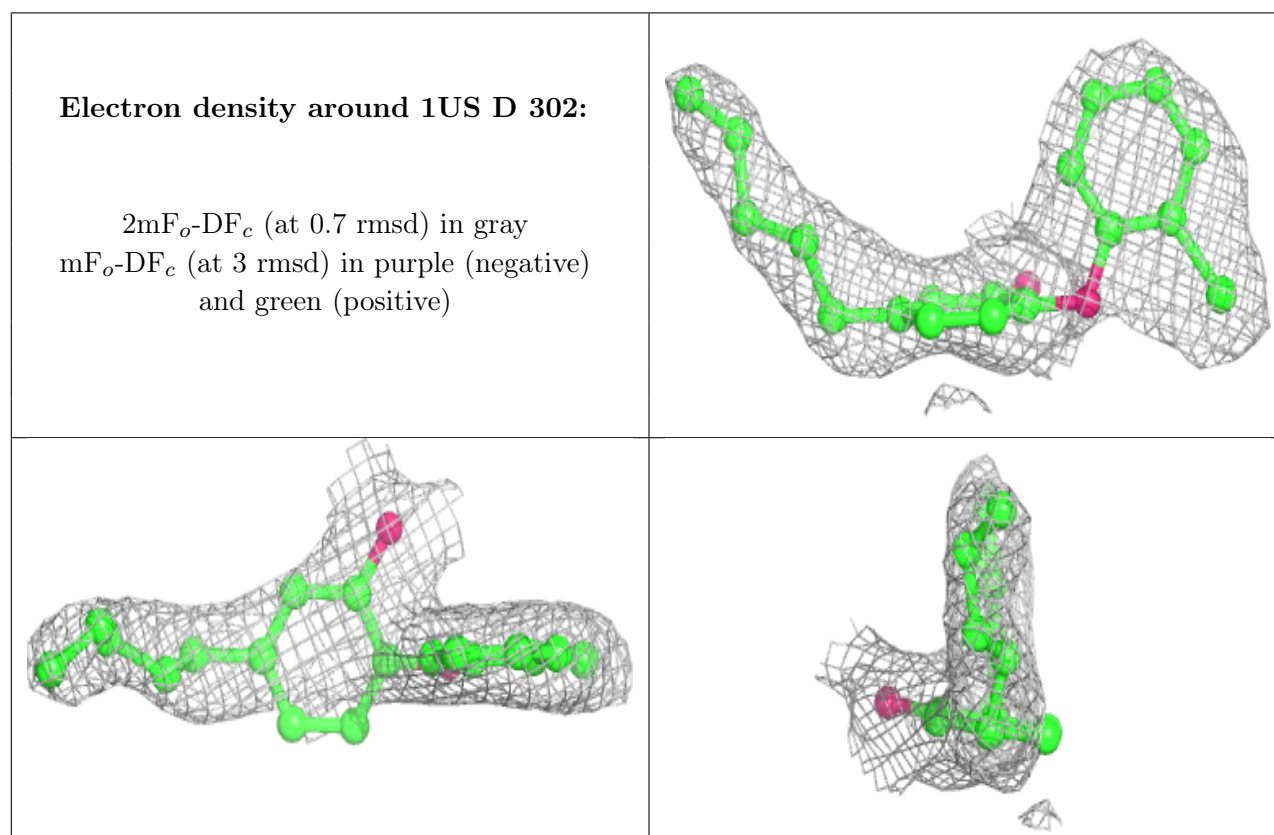
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	1US	D	302	20/21	0.88	0.26	52,59,75,78	0
2	NAD	D	301	44/44	0.93	0.19	54,65,76,103	0
3	1US	C	302	19/21	0.94	0.14	34,42,52,55	0
3	1US	B	302	20/21	0.95	0.13	31,36,42,48	0
3	1US	A	302	19/21	0.96	0.13	24,32,39,42	0

*Continued on next page...*

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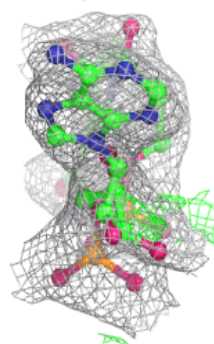
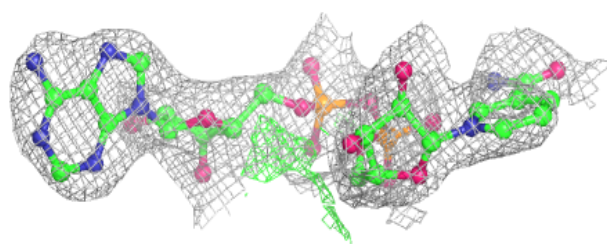
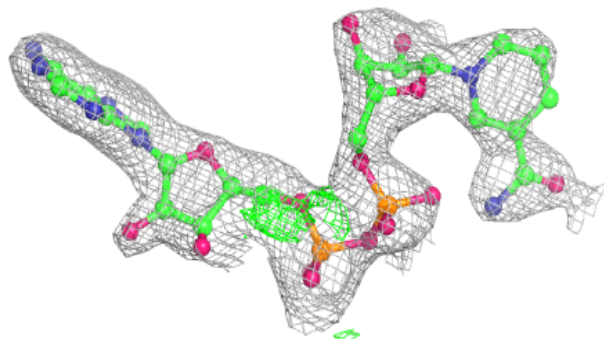
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAD	A	301	44/44	0.96	0.13	20,32,41,50	0
2	NAD	C	301	44/44	0.97	0.11	29,41,52,58	0
2	NAD	B	301	44/44	0.97	0.12	27,38,46,49	0

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.

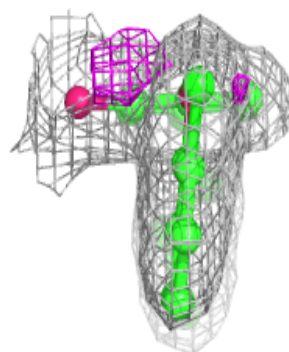
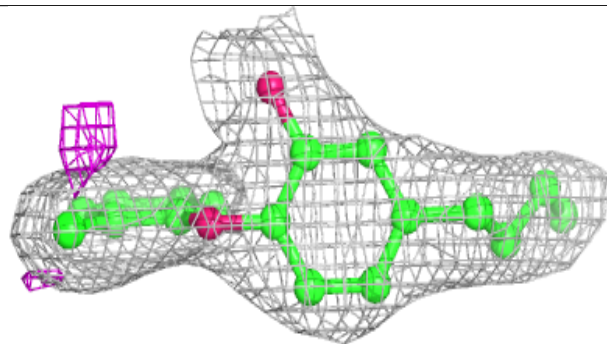


**Electron density around NAD D 301:**

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

**Electron density around 1US C 302:**

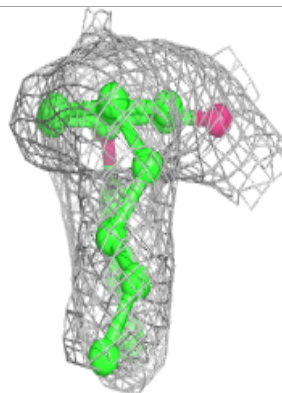
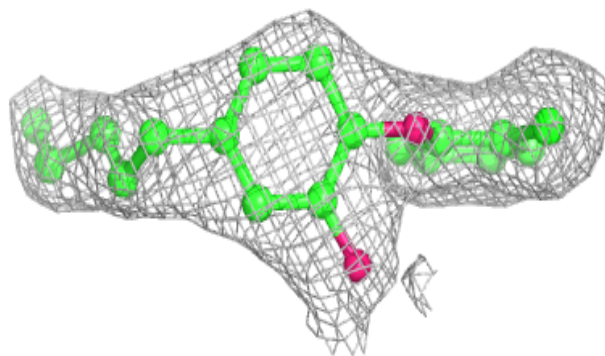
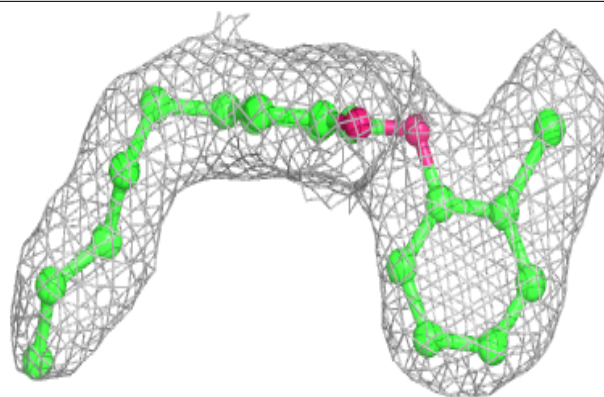
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



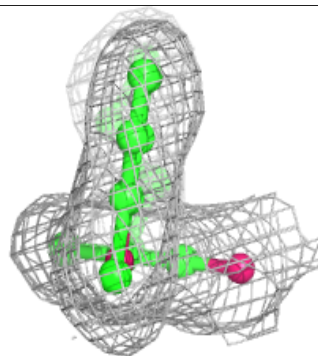
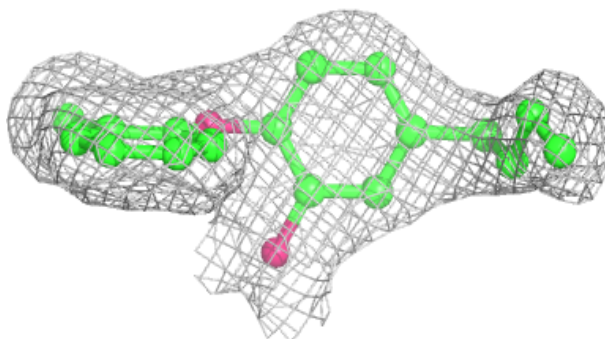
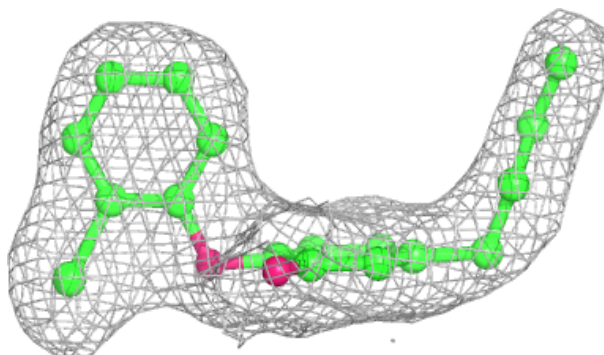


**Electron density around 1US B 302:**

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

**Electron density around 1US A 302:**

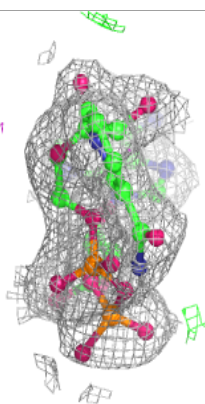
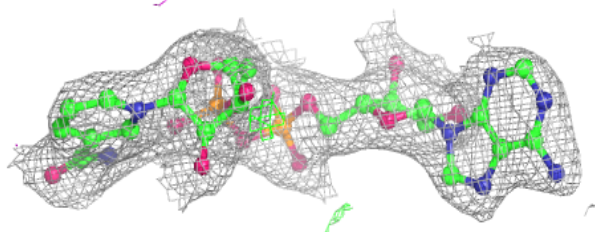
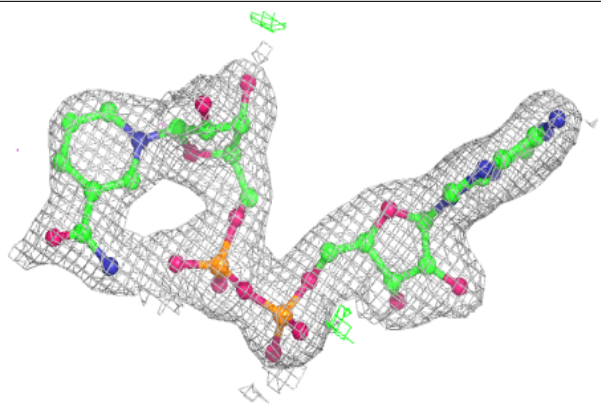
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



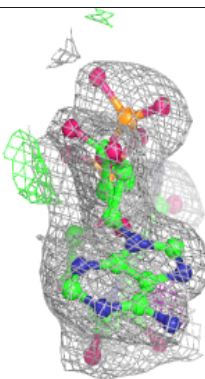
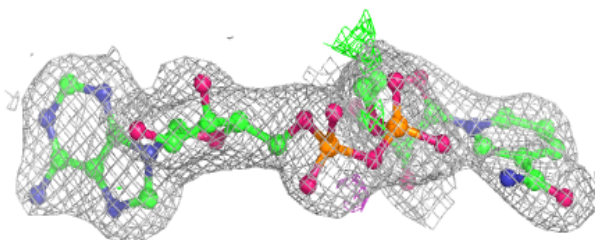
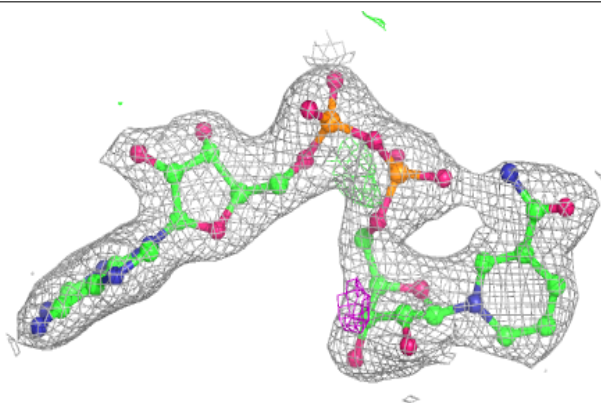


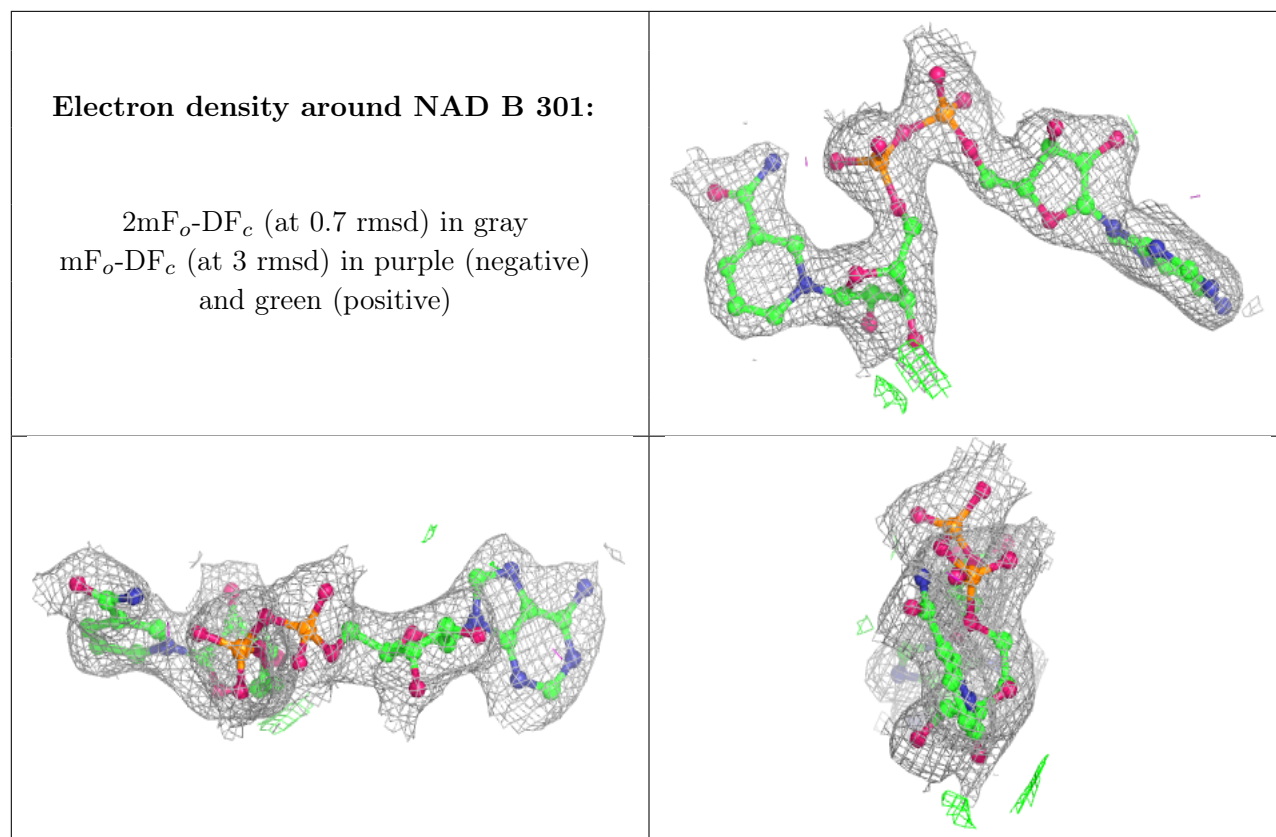
**Electron density around NAD A 301:**

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

**Electron density around NAD C 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 [i](#)

There are no such residues in this entry.