



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 12:36 PM EDT

PDB ID : 3LU1  
Title : Crystal Structure Analysis of WbgU: a UDP-GalNAc 4-epimerase  
Authors : Bhatt, V.S.; Guo, C.Y.; Zhao, G.; Yi, W.; Liu, Z.J.; Wang, P.G.  
Deposited on : 2010-02-16  
Resolution : 2.50 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>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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

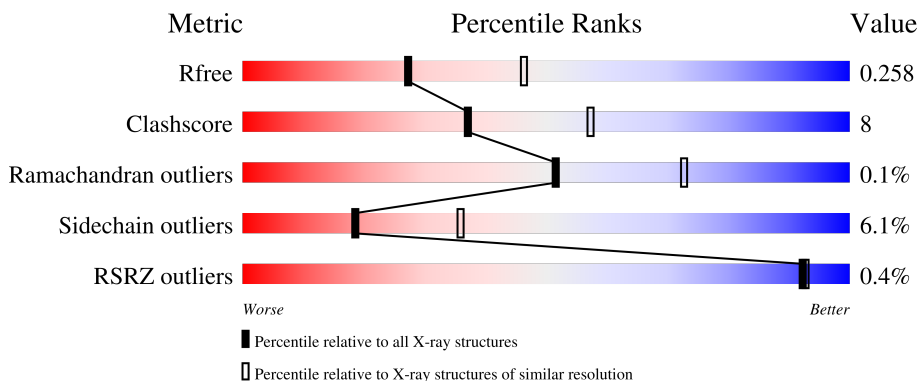
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	364	 76% 15% 8%
1	B	364	 73% 16% 8%
1	C	364	 75% 16% 8%
1	D	364	 74% 16% 8%

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
4	GLY	B	345	-	X	-	-

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 11231 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 WbgU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	336	Total 2681	C 1712	N 459	O 502	S 8	0	0	0
1	B	334	Total 2661	C 1698	N 457	O 499	S 7	0	0	0
1	C	334	Total 2661	C 1698	N 457	O 499	S 7	0	0	0
1	D	336	Total 2681	C 1712	N 459	O 502	S 8	0	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q7BJX9
A	-20	GLY	-	expression tag	UNP Q7BJX9
A	-19	SER	-	expression tag	UNP Q7BJX9
A	-18	SER	-	expression tag	UNP Q7BJX9
A	-17	HIS	-	expression tag	UNP Q7BJX9
A	-16	HIS	-	expression tag	UNP Q7BJX9
A	-15	HIS	-	expression tag	UNP Q7BJX9
A	-14	HIS	-	expression tag	UNP Q7BJX9
A	-13	HIS	-	expression tag	UNP Q7BJX9
A	-12	HIS	-	expression tag	UNP Q7BJX9
A	-11	SER	-	expression tag	UNP Q7BJX9
A	-10	SER	-	expression tag	UNP Q7BJX9
A	-9	GLY	-	expression tag	UNP Q7BJX9
A	-8	LEU	-	expression tag	UNP Q7BJX9
A	-7	VAL	-	expression tag	UNP Q7BJX9
A	-6	PRO	-	expression tag	UNP Q7BJX9
A	-5	ALA	-	expression tag	UNP Q7BJX9
A	-4	GLY	-	expression tag	UNP Q7BJX9
A	-3	SER	-	expression tag	UNP Q7BJX9
B	-21	MET	-	expression tag	UNP Q7BJX9
B	-20	GLY	-	expression tag	UNP Q7BJX9

*Continued on next page...*

*Continued from previous page...*

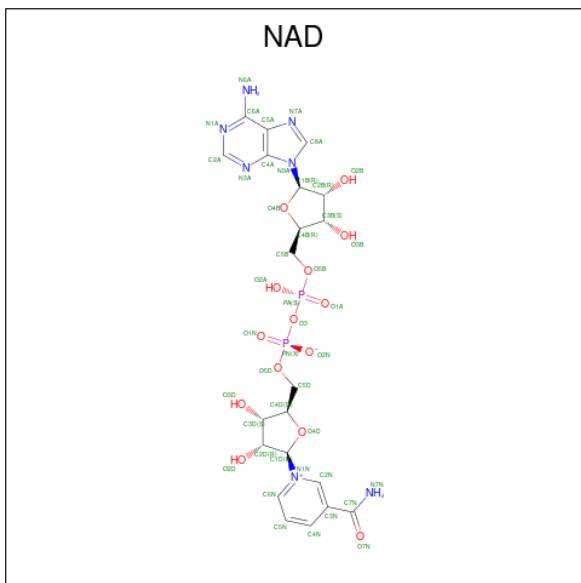
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	SER	-	expression tag	UNP Q7BJX9
B	-18	SER	-	expression tag	UNP Q7BJX9
B	-17	HIS	-	expression tag	UNP Q7BJX9
B	-16	HIS	-	expression tag	UNP Q7BJX9
B	-15	HIS	-	expression tag	UNP Q7BJX9
B	-14	HIS	-	expression tag	UNP Q7BJX9
B	-13	HIS	-	expression tag	UNP Q7BJX9
B	-12	HIS	-	expression tag	UNP Q7BJX9
B	-11	SER	-	expression tag	UNP Q7BJX9
B	-10	SER	-	expression tag	UNP Q7BJX9
B	-9	GLY	-	expression tag	UNP Q7BJX9
B	-8	LEU	-	expression tag	UNP Q7BJX9
B	-7	VAL	-	expression tag	UNP Q7BJX9
B	-6	PRO	-	expression tag	UNP Q7BJX9
B	-5	ALA	-	expression tag	UNP Q7BJX9
B	-4	GLY	-	expression tag	UNP Q7BJX9
B	-3	SER	-	expression tag	UNP Q7BJX9
C	-21	MET	-	expression tag	UNP Q7BJX9
C	-20	GLY	-	expression tag	UNP Q7BJX9
C	-19	SER	-	expression tag	UNP Q7BJX9
C	-18	SER	-	expression tag	UNP Q7BJX9
C	-17	HIS	-	expression tag	UNP Q7BJX9
C	-16	HIS	-	expression tag	UNP Q7BJX9
C	-15	HIS	-	expression tag	UNP Q7BJX9
C	-14	HIS	-	expression tag	UNP Q7BJX9
C	-13	HIS	-	expression tag	UNP Q7BJX9
C	-12	HIS	-	expression tag	UNP Q7BJX9
C	-11	SER	-	expression tag	UNP Q7BJX9
C	-10	SER	-	expression tag	UNP Q7BJX9
C	-9	GLY	-	expression tag	UNP Q7BJX9
C	-8	LEU	-	expression tag	UNP Q7BJX9
C	-7	VAL	-	expression tag	UNP Q7BJX9
C	-6	PRO	-	expression tag	UNP Q7BJX9
C	-5	ALA	-	expression tag	UNP Q7BJX9
C	-4	GLY	-	expression tag	UNP Q7BJX9
C	-3	SER	-	expression tag	UNP Q7BJX9
D	-21	MET	-	expression tag	UNP Q7BJX9
D	-20	GLY	-	expression tag	UNP Q7BJX9
D	-19	SER	-	expression tag	UNP Q7BJX9
D	-18	SER	-	expression tag	UNP Q7BJX9
D	-17	HIS	-	expression tag	UNP Q7BJX9
D	-16	HIS	-	expression tag	UNP Q7BJX9

*Continued on next page...*

Continued from previous page...

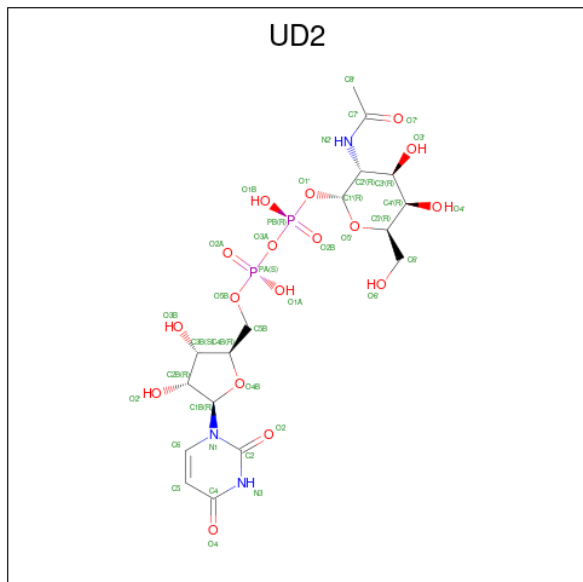
Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	HIS	-	expression tag	UNP Q7BJX9
D	-14	HIS	-	expression tag	UNP Q7BJX9
D	-13	HIS	-	expression tag	UNP Q7BJX9
D	-12	HIS	-	expression tag	UNP Q7BJX9
D	-11	SER	-	expression tag	UNP Q7BJX9
D	-10	SER	-	expression tag	UNP Q7BJX9
D	-9	GLY	-	expression tag	UNP Q7BJX9
D	-8	LEU	-	expression tag	UNP Q7BJX9
D	-7	VAL	-	expression tag	UNP Q7BJX9
D	-6	PRO	-	expression tag	UNP Q7BJX9
D	-5	ALA	-	expression tag	UNP Q7BJX9
D	-4	GLY	-	expression tag	UNP Q7BJX9
D	-3	SER	-	expression tag	UNP Q7BJX9

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



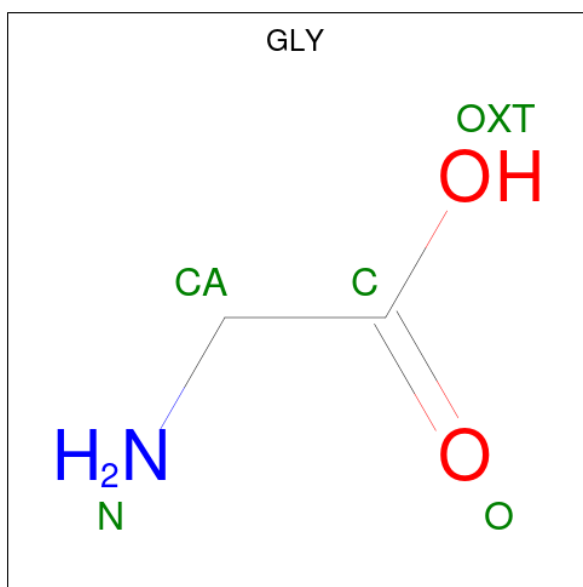
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is URIDINE-DIPHOSPHATE-N-ACETYLGLACTOSAMINE (three-letter code: UD2) (formula:  $C_{17}H_{27}N_3O_{17}P_2$ ).



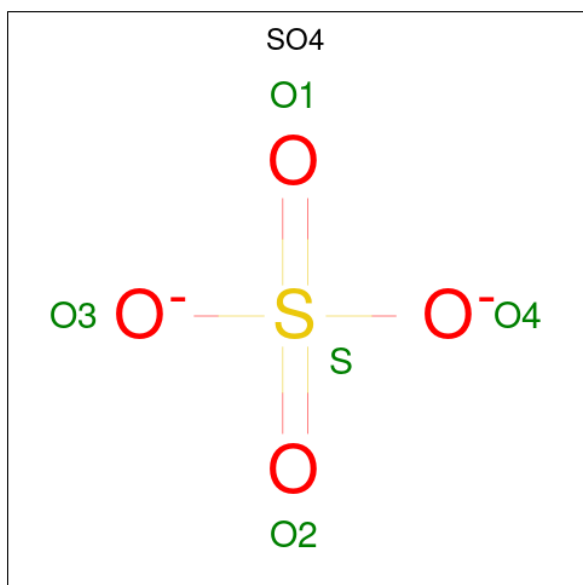
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	D	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 4 is GLYCINE (three-letter code: GLY) (formula:  $C_2H_5NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	5	2	1	2	0	0
4	B	1	5	2	1	2	0	0
4	C	1	5	2	1	2	0	0
4	D	1	5	2	1	2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Na 1 1	0	0

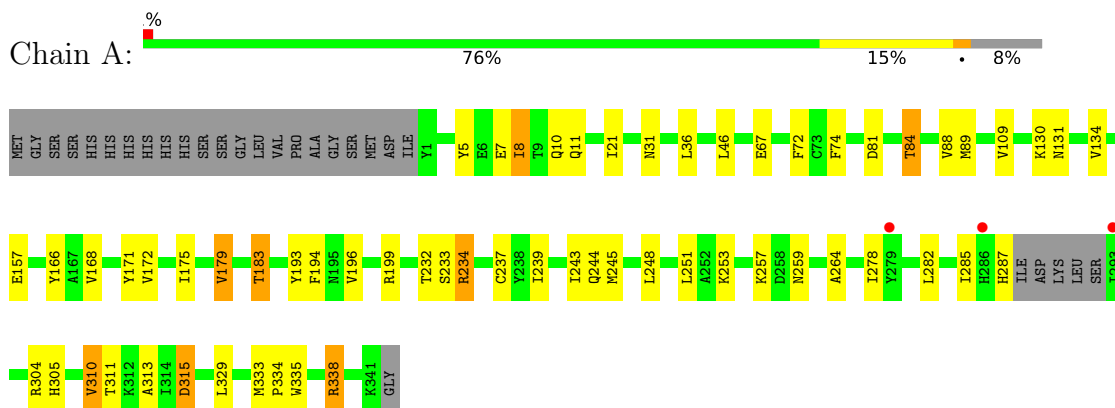
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	46	Total O 46 46	0	0
7	B	57	Total O 57 57	0	0
7	C	42	Total O 42 42	0	0
7	D	34	Total O 34 34	0	0

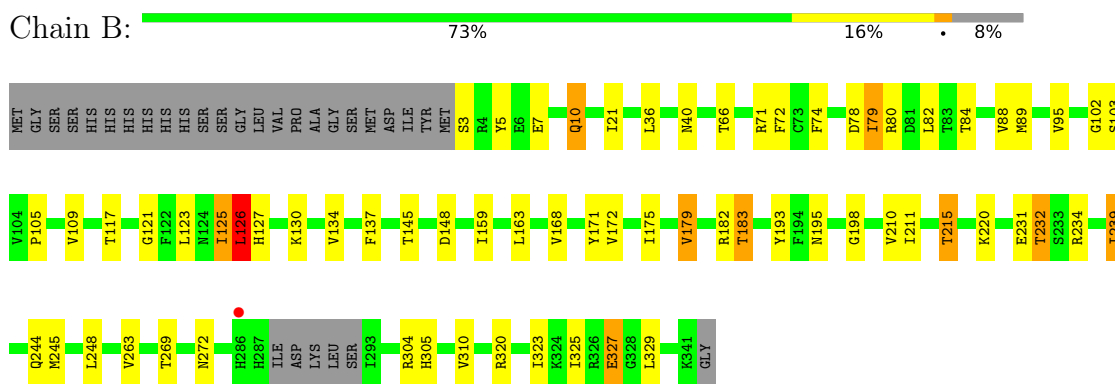
### 3 Residue-property plots

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.

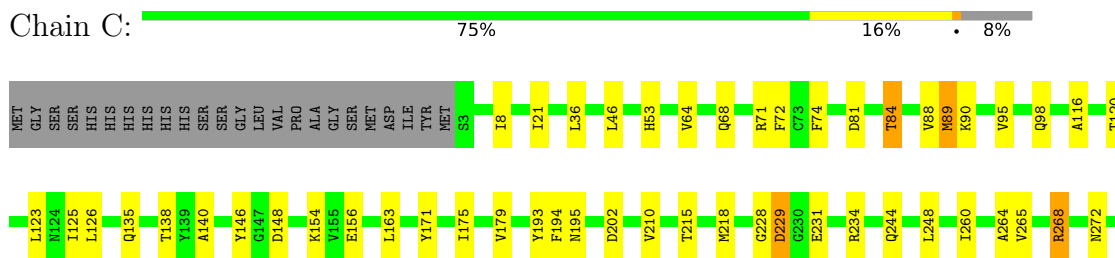
- Molecule 1: WbgU



- Molecule 1: WbgU



- Molecule 1: WbgU





- Molecule 1: WbgU

Chain D: 74% 16% 8%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.13Å 78.13Å 231.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.03 – 2.50 44.03 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.7 (44.03-2.50) 94.7 (44.03-2.50)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.51Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.204 , 0.258 0.203 , 0.258	Depositor DCC
$R_{free}$ test set	2637 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 7.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for -h,-k,l 0.469 for h,-h-k,-l 0.017 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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: SO4, NAD, UD2, NA

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	0.39	0/2739	0.54	0/3717
1	B	0.40	0/2718	0.56	1/3689 (0.0%)
1	C	0.41	0/2718	0.53	0/3689
1	D	0.39	0/2739	0.54	0/3717
All	All	0.40	0/10914	0.54	1/14812 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	LEU	CA-CB-CG	6.53	130.33	115.30

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	2681	0	2658	41	0
1	B	2661	0	2637	41	0
1	C	2661	0	2637	38	0
1	D	2681	0	2658	47	0
2	A	44	0	26	3	0
2	B	44	0	26	4	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	44	0	26	2	0
2	D	44	0	26	5	0
3	A	39	0	25	3	0
3	B	39	0	25	4	0
3	C	39	0	25	1	0
3	D	39	0	25	5	0
4	A	5	0	2	0	0
4	B	5	0	2	0	0
4	C	5	0	2	0	0
4	D	5	0	2	0	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
6	D	1	0	0	0	0
7	A	46	0	0	4	0
7	B	57	0	0	0	0
7	C	42	0	0	0	0
7	D	34	0	0	1	0
All	All	11231	0	10802	170	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 8.

All (170) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:MET:HE1	1:A:134:VAL:HG11	1.56	0.87
1:C:244:GLN:HE22	1:C:320:ARG:H	1.21	0.85
1:B:244:GLN:HE22	1:B:320:ARG:H	1.29	0.80
1:B:211:ILE:O	1:B:215:THR:HG23	1.81	0.80
2:B:343:NAD:C4N	3:B:344:UD2:H4'	2.12	0.79
1:C:229:ASP:HB3	1:C:231:GLU:H	1.46	0.79
2:C:343:NAD:C4N	3:C:344:UD2:H4'	2.15	0.77
1:D:179:VAL:O	1:D:183:THR:HG22	1.83	0.77
2:D:344:NAD:C4N	3:D:343:UD2:H4'	2.14	0.76
1:D:244:GLN:HE22	1:D:320:ARG:H	1.30	0.76
1:C:193:TYR:HB2	2:C:343:NAD:C5N	2.19	0.72
1:B:79:ILE:HD11	1:B:125:ILE:HD13	1.71	0.71
1:B:79:ILE:HG23	1:B:121:GLY:HA3	1.73	0.70
1:D:244:GLN:NE2	1:D:320:ARG:H	1.90	0.69
2:A:343:NAD:C4N	3:A:344:UD2:H4'	2.23	0.69
1:C:310:VAL:HG12	1:C:310:VAL:O	1.91	0.69

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:TYR:CE2	1:D:175:ILE:HD11	2.28	0.69
1:B:193:TYR:HB2	2:B:343:NAD:C5N	2.24	0.68
1:C:215:THR:HG23	1:C:333:MET:HE1	1.77	0.67
1:D:310:VAL:O	1:D:310:VAL:HG12	1.95	0.66
1:A:21:ILE:HD11	1:A:36:LEU:HD12	1.78	0.65
1:B:179:VAL:O	1:B:183:THR:HG23	1.97	0.64
1:D:78:ASP:OD1	1:D:80:ARG:HD3	1.98	0.63
1:A:282:LEU:O	1:A:285:ILE:HG22	1.99	0.62
1:D:61:LYS:HD2	1:D:69:TRP:CE2	2.33	0.62
1:A:179:VAL:O	1:A:183:THR:HG23	1.99	0.61
1:D:80:ARG:HD2	1:D:117:THR:HG22	1.83	0.61
1:B:82:LEU:HD22	1:D:112:ILE:HD13	1.81	0.61
1:C:64:VAL:HG13	1:C:68:GLN:HB2	1.82	0.60
1:C:148:ASP:HB3	1:C:163:LEU:HD21	1.85	0.59
1:C:310:VAL:O	1:C:310:VAL:CG1	2.51	0.59
1:A:89:MET:CE	1:A:134:VAL:HG11	2.32	0.58
1:A:11:GLN:NE2	1:D:205:GLY:HA2	2.19	0.58
1:A:171:TYR:CE2	1:A:175:ILE:HD11	2.38	0.57
1:A:31:ASN:HB3	1:A:243:ILE:HD11	1.86	0.57
1:B:7:GLU:O	1:B:10:GLN:HG3	2.04	0.56
1:C:53:HIS:NE2	1:C:202:ASP:OD2	2.35	0.56
1:A:278:ILE:O	7:A:361:HOH:O	2.17	0.56
1:A:7:GLU:OE1	1:D:106:ARG:NH1	2.39	0.56
1:D:94:HIS:ND1	1:D:136:SER:HB3	2.21	0.56
1:D:193:TYR:HB2	2:D:344:NAD:C5N	2.36	0.56
1:B:323:ILE:HG23	1:B:327:GLU:HG3	1.87	0.55
1:B:79:ILE:HG23	1:B:121:GLY:CA	2.37	0.55
1:B:21:ILE:HD11	1:B:36:LEU:HD12	1.88	0.55
1:B:78:ASP:OD1	1:B:80:ARG:HD3	2.07	0.54
1:B:168:VAL:O	1:B:172:VAL:HG23	2.06	0.54
1:B:244:GLN:HE21	1:B:248:LEU:HD11	1.73	0.54
1:C:21:ILE:HD11	1:C:36:LEU:HD12	1.89	0.54
1:C:218:MET:HE1	1:C:279:TYR:HA	1.90	0.53
1:C:265:VAL:HG11	1:C:324:LYS:HG2	1.89	0.53
1:B:126:LEU:HB3	1:B:137:PHE:CZ	2.44	0.53
1:C:81:ASP:HB2	1:C:84:THR:HG23	1.90	0.53
1:C:98:GLN:NE2	1:C:193:TYR:OH	2.40	0.53
1:C:116:ALA:O	1:C:120:THR:HB	2.07	0.53
1:D:146:TYR:CG	1:D:154:LYS:HD3	2.44	0.53
1:B:80:ARG:HD2	1:B:117:THR:HG22	1.90	0.52
1:A:334:PRO:O	1:A:338:ARG:HD3	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:THR:HG22	1:D:159:ILE:HD12	1.90	0.52
1:B:148:ASP:HB3	1:B:163:LEU:HD21	1.91	0.52
1:D:310:VAL:HG11	1:D:319:TYR:CE2	2.44	0.52
1:C:81:ASP:HB2	1:C:84:THR:CG2	2.40	0.52
1:A:81:ASP:OD2	1:A:84:THR:HG22	2.11	0.51
1:B:171:TYR:CE2	1:B:175:ILE:HD11	2.45	0.51
1:C:98:GLN:NE2	1:C:140:ALA:HB2	2.26	0.50
1:D:211:ILE:O	1:D:215:THR:HG23	2.10	0.50
1:B:310:VAL:CG1	1:B:310:VAL:O	2.59	0.50
1:C:244:GLN:NE2	1:C:320:ARG:H	1.98	0.50
1:A:81:ASP:HB3	1:A:84:THR:CG2	2.42	0.50
1:B:310:VAL:O	1:B:310:VAL:HG12	2.11	0.49
1:A:67:GLU:HB2	7:A:385:HOH:O	2.10	0.49
1:B:232:THR:HG22	1:B:304:ARG:HH11	1.78	0.49
1:A:8:ILE:HG23	1:A:251:LEU:HD22	1.95	0.49
1:A:193:TYR:HB2	2:A:343:NAD:C5N	2.42	0.49
1:C:194:PHE:HB2	1:C:264:ALA:HB2	1.95	0.49
1:A:194:PHE:HB2	1:A:264:ALA:HB2	1.95	0.49
1:C:218:MET:CE	1:C:279:TYR:HA	2.41	0.49
1:C:171:TYR:CE2	1:C:175:ILE:HD11	2.48	0.49
1:C:171:TYR:CZ	1:C:175:ILE:HD11	2.48	0.48
1:D:79:ILE:HG22	1:D:125:ILE:HD11	1.95	0.48
1:A:310:VAL:O	1:A:310:VAL:CG1	2.62	0.48
1:B:72:PHE:CZ	1:B:74:PHE:HB2	2.48	0.48
1:D:102:GLY:O	1:D:103:SER:HB3	2.13	0.48
2:D:344:NAD:C4N	3:D:343:UD2:C4'	2.90	0.48
1:A:10:GLN:NE2	1:D:106:ARG:HD3	2.29	0.47
1:B:127:HIS:ND1	1:D:112:ILE:HD11	2.28	0.47
1:B:79:ILE:HD11	1:B:125:ILE:CD1	2.43	0.47
1:B:89:MET:HE2	1:B:134:VAL:HG21	1.96	0.47
1:B:123:LEU:HD12	1:B:126:LEU:HD11	1.96	0.47
1:A:278:ILE:C	7:A:361:HOH:O	2.52	0.47
1:D:21:ILE:HD11	1:D:36:LEU:HD12	1.97	0.47
1:D:286:HIS:CD2	1:D:287:HIS:H	2.32	0.47
1:D:187:LYS:NZ	7:D:354:HOH:O	2.47	0.47
1:D:310:VAL:O	1:D:310:VAL:CG1	2.62	0.47
3:B:344:UD2:O1B	3:B:344:UD2:H5'1	2.14	0.46
1:C:72:PHE:CZ	1:C:74:PHE:HB2	2.50	0.46
1:B:195:ASN:ND2	1:B:234:ARG:HD2	2.30	0.46
1:B:40:ASN:O	1:B:71:ARG:NH1	2.49	0.46
1:B:105:PRO:O	1:B:109:VAL:HG23	2.15	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ASP:HB2	1:D:161:ASN:H	1.80	0.46
1:B:182:ARG:HD3	1:D:163:LEU:HD23	1.96	0.46
1:B:239:ILE:H	1:B:239:ILE:HG13	1.43	0.46
1:D:210:VAL:HG22	3:D:343:UD2:H5'2	1.97	0.45
2:D:344:NAD:H4N	3:D:343:UD2:H4'	1.95	0.45
1:A:168:VAL:O	1:A:172:VAL:HG23	2.15	0.45
1:D:20:LEU:HD13	1:D:88:VAL:HG13	1.97	0.45
1:D:194:PHE:HB2	1:D:264:ALA:HB2	1.97	0.45
1:A:179:VAL:O	1:A:183:THR:CG2	2.63	0.45
2:B:343:NAD:C4N	3:B:344:UD2:C4'	2.91	0.45
1:C:310:VAL:HG11	1:C:319:TYR:HE2	1.82	0.45
1:B:89:MET:HE1	1:B:95:VAL:HG22	1.99	0.45
1:A:89:MET:HE1	1:A:134:VAL:CG1	2.39	0.45
1:A:257:LYS:O	1:A:259:ASN:ND2	2.44	0.45
1:B:102:GLY:O	1:B:103:SER:HB3	2.17	0.45
1:D:310:VAL:HG11	1:D:319:TYR:HE2	1.81	0.45
1:B:145:THR:HG22	1:B:159:ILE:HD12	1.98	0.45
2:B:343:NAD:H4N	3:B:344:UD2:H4'	1.93	0.45
1:A:329:LEU:O	1:A:333:MET:HG2	2.18	0.44
1:A:196:VAL:HA	1:A:237:CYS:O	2.18	0.44
1:A:285:ILE:HG23	1:A:287:HIS:HD2	1.82	0.44
1:A:10:GLN:HE22	1:D:106:ARG:HD3	1.83	0.44
1:A:72:PHE:CZ	1:A:74:PHE:HB2	2.53	0.44
1:C:215:THR:HG23	1:C:333:MET:CE	2.47	0.44
1:D:286:HIS:CG	1:D:287:HIS:H	2.35	0.44
1:A:166:TYR:HE2	3:A:344:UD2:HO4'	1.65	0.44
1:A:282:LEU:N	7:A:361:HOH:O	2.51	0.44
1:C:268:ARG:HG3	1:C:307:GLN:HB2	2.00	0.44
1:A:304:ARG:HG3	1:A:305:HIS:CD2	2.53	0.44
1:D:195:ASN:ND2	1:D:234:ARG:HD2	2.32	0.44
1:C:310:VAL:HG11	1:C:319:TYR:CE2	2.53	0.43
1:A:233:SER:O	1:A:234:ARG:HD3	2.18	0.43
1:D:84:THR:O	1:D:88:VAL:HB	2.19	0.43
1:A:81:ASP:O	1:A:84:THR:HG23	2.19	0.43
1:A:89:MET:CE	1:A:134:VAL:CG1	2.96	0.43
1:A:130:LYS:NZ	1:A:131:ASN:OD1	2.52	0.43
1:C:244:GLN:HE21	1:C:248:LEU:HD11	1.83	0.43
1:A:232:THR:HG23	1:A:304:ARG:O	2.19	0.43
1:C:8:ILE:HD12	1:C:248:LEU:HD23	2.01	0.43
1:C:156:GLU:HG2	1:C:260:ILE:O	2.19	0.43
1:B:304:ARG:HG3	1:B:305:HIS:CD2	2.53	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:TYR:CG	1:B:244:GLN:HG3	2.54	0.43
1:C:304:ARG:HG3	1:C:305:HIS:CD2	2.54	0.42
1:C:325:ILE:H	1:C:325:ILE:HG13	1.38	0.42
1:D:81:ASP:HB3	1:D:84:THR:HG23	2.01	0.42
2:A:343:NAD:C4N	3:A:344:UD2:C4'	2.94	0.42
1:A:311:THR:O	1:A:315:ASP:HB2	2.19	0.42
1:B:231:GLU:OE2	1:B:272:ASN:ND2	2.53	0.42
1:B:198:GLY:HA3	1:B:239:ILE:HG12	2.02	0.42
1:C:228:GLY:N	1:C:296:ARG:O	2.50	0.42
1:A:245:MET:HE1	1:A:313:ALA:HB1	2.02	0.42
1:B:323:ILE:HG23	1:B:327:GLU:CG	2.50	0.42
1:C:195:ASN:ND2	1:C:234:ARG:HD2	2.35	0.42
1:D:210:VAL:HG13	3:D:343:UD2:C6	2.50	0.42
1:C:89:MET:HE1	1:C:95:VAL:CG2	2.50	0.41
1:D:81:ASP:HB3	1:D:84:THR:CG2	2.50	0.41
1:B:245:MET:HG3	1:B:263:VAL:HG13	2.03	0.41
1:C:320:ARG:HD2	1:C:320:ARG:HA	1.82	0.41
1:D:79:ILE:HG12	2:D:344:NAD:C6A	2.50	0.41
1:C:231:GLU:OE2	1:C:272:ASN:ND2	2.54	0.41
1:D:89:MET:HE2	1:D:95:VAL:HG22	2.03	0.41
1:D:5:TYR:OH	1:D:35:LYS:HD3	2.21	0.41
1:A:5:TYR:CG	1:A:244:GLN:HG3	2.56	0.41
1:A:199:ARG:HH21	1:A:335:TRP:HB2	1.86	0.41
1:C:146:TYR:CD1	1:C:154:LYS:HD2	2.56	0.41
1:D:89:MET:HE2	1:D:134:VAL:HG21	2.03	0.41
1:D:89:MET:CE	1:D:95:VAL:HG22	2.51	0.41
1:B:159:ILE:HD13	1:B:159:ILE:HA	1.86	0.40
1:D:72:PHE:CZ	1:D:74:PHE:HB2	2.56	0.40
1:D:170:LYS:HD3	1:D:170:LYS:HA	1.94	0.40
1:D:89:MET:HE2	1:D:95:VAL:CG2	2.52	0.40
1:D:239:ILE:H	1:D:239:ILE:HG13	1.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/364 (91%)	317 (96%)	15 (4%)	0	100	100
1	B	330/364 (91%)	315 (96%)	15 (4%)	0	100	100
1	C	330/364 (91%)	314 (95%)	16 (5%)	0	100	100
1	D	332/364 (91%)	313 (94%)	18 (5%)	1 (0%)	41	61
All	All	1324/1456 (91%)	1259 (95%)	64 (5%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	103	SER

### 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	290/313 (93%)	275 (95%)	15 (5%)	23	44
1	B	288/313 (92%)	268 (93%)	20 (7%)	15	30
1	C	288/313 (92%)	272 (94%)	16 (6%)	21	40
1	D	290/313 (93%)	270 (93%)	20 (7%)	15	30
All	All	1156/1252 (92%)	1085 (94%)	71 (6%)	18	36

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	46	LEU
1	A	84	THR
1	A	88	VAL
1	A	109	VAL
1	A	157	GLU
1	A	179	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	183	THR
1	A	234	ARG
1	A	239	ILE
1	A	248	LEU
1	A	253	LYS
1	A	310	VAL
1	A	315	ASP
1	A	338	ARG
1	B	3	SER
1	B	10	GLN
1	B	66	THR
1	B	79	ILE
1	B	84	THR
1	B	88	VAL
1	B	125	ILE
1	B	126	LEU
1	B	130	LYS
1	B	179	VAL
1	B	183	THR
1	B	210	VAL
1	B	215	THR
1	B	220	LYS
1	B	232	THR
1	B	239	ILE
1	B	269	THR
1	B	325	ILE
1	B	327	GLU
1	B	329	LEU
1	C	46	LEU
1	C	71	ARG
1	C	84	THR
1	C	88	VAL
1	C	89	MET
1	C	90	LYS
1	C	123	LEU
1	C	125	ILE
1	C	126	LEU
1	C	135	GLN
1	C	138	THR
1	C	179	VAL
1	C	210	VAL
1	C	229	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	268	ARG
1	C	325	ILE
1	D	35	LYS
1	D	83	THR
1	D	84	THR
1	D	126	LEU
1	D	130	LYS
1	D	134	VAL
1	D	136	SER
1	D	154	LYS
1	D	155	VAL
1	D	157	GLU
1	D	183	THR
1	D	210	VAL
1	D	232	THR
1	D	239	ILE
1	D	242	VAL
1	D	299	ARG
1	D	326	ARG
1	D	329	LEU
1	D	338	ARG
1	D	341	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	11	GLN
1	A	287	HIS
1	B	11	GLN
1	B	98	GLN
1	B	173	ASN
1	B	195	ASN
1	B	244	GLN
1	B	287	HIS
1	C	98	GLN
1	C	195	ASN
1	C	244	GLN
1	D	127	HIS
1	D	195	ASN
1	D	244	GLN
1	D	286	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

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	UD2	C	344	-	38,41,41	0.94	1 (2%)	57,62,62	1.52	6 (10%)
4	GLY	D	348	-	4,4,4	1.10	1 (25%)	3,4,4	1.75	1 (33%)
2	NAD	D	344	-	42,48,48	1.31	4 (9%)	50,73,73	1.30	6 (12%)
2	NAD	C	343	-	42,48,48	1.29	4 (9%)	50,73,73	1.20	4 (8%)
5	SO4	C	345	-	4,4,4	0.16	0	6,6,6	0.13	0
4	GLY	A	345	-	4,4,4	1.05	1 (25%)	3,4,4	1.69	1 (33%)
5	SO4	D	347	-	4,4,4	0.15	0	6,6,6	0.11	0
5	SO4	D	346	-	4,4,4	0.12	0	6,6,6	0.14	0
2	NAD	B	343	-	42,48,48	1.29	4 (9%)	50,73,73	1.17	5 (10%)
4	GLY	B	345	-	4,4,4	1.08	1 (25%)	3,4,4	1.84	2 (66%)
4	GLY	C	346	-	4,4,4	1.22	1 (25%)	3,4,4	1.90	1 (33%)
3	UD2	D	343	-	38,41,41	1.00	1 (2%)	57,62,62	1.41	7 (12%)
3	UD2	A	344	-	38,41,41	0.90	1 (2%)	57,62,62	1.40	6 (10%)
2	NAD	A	343	-	42,48,48	1.30	4 (9%)	50,73,73	1.28	5 (10%)
3	UD2	B	344	-	38,41,41	0.92	1 (2%)	57,62,62	1.46	8 (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
3	UD2	C	344	-	-	2/26/63/63	0/3/3/3
4	GLY	D	348	-	-	0/2/2/2	-
2	NAD	D	344	-	-	8/26/62/62	0/5/5/5
2	NAD	C	343	-	-	9/26/62/62	0/5/5/5
4	GLY	A	345	-	-	0/2/2/2	-
2	NAD	B	343	-	-	10/26/62/62	0/5/5/5
4	GLY	B	345	-	-	2/2/2/2	-
4	GLY	C	346	-	-	0/2/2/2	-
3	UD2	D	343	-	-	11/26/63/63	0/3/3/3
3	UD2	A	344	-	-	5/26/63/63	0/3/3/3
2	NAD	A	343	-	-	10/26/62/62	0/5/5/5
3	UD2	B	344	-	-	3/26/63/63	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	343	NAD	C2N-N1N	5.27	1.41	1.35
2	C	343	NAD	C2N-N1N	4.92	1.40	1.35
2	A	343	NAD	C2N-N1N	4.67	1.40	1.35
2	D	344	NAD	C2N-N1N	4.54	1.40	1.35
2	D	344	NAD	O4D-C1D	3.89	1.46	1.41
2	A	343	NAD	O4D-C1D	3.83	1.46	1.41
2	C	343	NAD	O4D-C1D	3.63	1.46	1.41
2	B	343	NAD	O4D-C1D	3.24	1.45	1.41
2	D	344	NAD	O4B-C1B	2.88	1.45	1.41
2	B	343	NAD	C3N-C7N	2.40	1.54	1.50
4	C	346	GLY	OXT-C	-2.36	1.22	1.30
2	C	343	NAD	C6N-N1N	2.29	1.41	1.35
3	C	344	UD2	C2-N1	2.28	1.42	1.38
2	A	343	NAD	C6N-N1N	2.26	1.40	1.35
2	A	343	NAD	O4B-C1B	2.23	1.44	1.41
2	D	344	NAD	C6N-N1N	2.23	1.40	1.35
2	C	343	NAD	C3N-C7N	2.21	1.53	1.50
2	B	343	NAD	C6N-N1N	2.18	1.40	1.35
3	D	343	UD2	C6-C5	2.15	1.40	1.35
4	D	348	GLY	OXT-C	-2.12	1.23	1.30
4	B	345	GLY	OXT-C	-2.08	1.23	1.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	344	UD2	C6-C5	2.07	1.39	1.35
3	A	344	UD2	C6-C5	2.06	1.39	1.35
4	A	345	GLY	OXT-C	-2.01	1.24	1.30

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	344	NAD	N3A-C2A-N1A	-5.05	120.79	128.68
2	A	343	NAD	N3A-C2A-N1A	-5.03	120.82	128.68
3	A	344	UD2	C4-N3-C2	-4.88	120.15	126.58
3	D	343	UD2	C4-N3-C2	-4.76	120.30	126.58
3	C	344	UD2	C4-N3-C2	-4.73	120.34	126.58
3	B	344	UD2	C4-N3-C2	-4.72	120.36	126.58
3	C	344	UD2	O5'-C1'-O1'	-4.70	105.22	111.36
2	C	343	NAD	N3A-C2A-N1A	-4.69	121.35	128.68
2	B	343	NAD	N3A-C2A-N1A	-4.27	122.01	128.68
3	A	344	UD2	C5-C4-N3	3.84	120.58	114.84
3	D	343	UD2	C5-C4-N3	3.74	120.44	114.84
3	B	344	UD2	N3-C2-N1	3.66	119.75	114.89
3	A	344	UD2	N3-C2-N1	3.65	119.73	114.89
3	C	344	UD2	C5-C4-N3	3.61	120.25	114.84
3	B	344	UD2	O3A-PB-O1'	-3.51	95.42	102.48
3	D	343	UD2	N3-C2-N1	3.49	119.53	114.89
3	B	344	UD2	C5-C4-N3	3.36	119.87	114.84
3	C	344	UD2	O3A-PB-O1'	-3.34	95.75	102.48
3	C	344	UD2	O4-C4-C5	-3.27	119.41	125.16
3	D	343	UD2	PB-O3A-PA	-3.08	122.26	132.83
2	D	344	NAD	C3N-C7N-N7N	-3.03	114.12	117.75
3	D	343	UD2	O4-C4-C5	-2.97	119.94	125.16
3	C	344	UD2	N3-C2-N1	2.96	118.81	114.89
2	A	343	NAD	O4D-C1D-C2D	-2.96	102.61	106.93
3	A	344	UD2	O4-C4-C5	-2.81	120.22	125.16
3	A	344	UD2	O3A-PB-O1'	-2.76	96.91	102.48
2	D	344	NAD	O4D-C1D-C2D	-2.76	102.89	106.93
4	C	346	GLY	OXT-C-O	-2.66	116.67	123.30
3	D	343	UD2	O5'-C5'-C4'	-2.66	104.87	109.69
2	A	343	NAD	C3N-C7N-N7N	-2.58	114.66	117.75
3	B	344	UD2	O4-C4-C5	-2.55	120.67	125.16
2	A	343	NAD	C3D-C2D-C1D	-2.50	97.21	100.98
4	B	345	GLY	OXT-C-O	-2.42	117.27	123.30
3	B	344	UD2	C6'-C5'-C4'	-2.40	107.38	113.00
3	B	344	UD2	O5'-C1'-O1'	-2.40	108.23	111.36

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	343	NAD	O4B-C1B-C2B	-2.37	103.47	106.93
4	D	348	GLY	OXT-C-O	-2.36	117.41	123.30
3	D	343	UD2	C1'-O5'-C5'	-2.31	109.15	113.69
2	C	343	NAD	O4D-C1D-C2D	-2.30	103.56	106.93
2	B	343	NAD	C3D-C2D-C1D	-2.28	97.54	100.98
2	D	344	NAD	C3D-C2D-C1D	-2.28	97.55	100.98
2	A	343	NAD	PN-O3-PA	-2.24	125.14	132.83
4	A	345	GLY	OXT-C-O	-2.23	117.74	123.30
2	D	344	NAD	PN-O3-PA	-2.22	125.21	132.83
3	B	344	UD2	C4'-C3'-C2'	2.15	113.49	110.34
2	B	343	NAD	PN-O3-PA	-2.09	125.66	132.83
3	A	344	UD2	PB-O3A-PA	-2.09	125.67	132.83
2	C	343	NAD	O4B-C1B-C2B	-2.08	103.89	106.93
2	D	344	NAD	O4B-C1B-C2B	-2.08	103.89	106.93
4	B	345	GLY	OXT-C-CA	2.06	121.63	113.45
2	C	343	NAD	C3N-C7N-N7N	-2.04	115.30	117.75
2	B	343	NAD	C3N-C7N-N7N	-2.01	115.34	117.75

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	343	NAD	C5B-O5B-PA-O2A
2	A	343	NAD	C5D-O5D-PN-O1N
2	B	343	NAD	C5B-O5B-PA-O2A
2	B	343	NAD	PN-O3-PA-O5B
2	B	343	NAD	C5D-O5D-PN-O1N
2	C	343	NAD	C5B-O5B-PA-O2A
2	C	343	NAD	PN-O3-PA-O5B
2	C	343	NAD	C5D-O5D-PN-O3
2	C	343	NAD	C5D-O5D-PN-O2N
2	C	343	NAD	O4D-C1D-N1N-C2N
2	D	344	NAD	C5B-O5B-PA-O2A
2	D	344	NAD	C5D-O5D-PN-O3
2	D	344	NAD	C5D-O5D-PN-O2N
3	A	344	UD2	PB-O3A-PA-O5B
3	B	344	UD2	PB-O3A-PA-O5B
3	C	344	UD2	C5B-O5B-PA-O2A
3	D	343	UD2	C5B-O5B-PA-O2A
3	D	343	UD2	PB-O3A-PA-O5B
4	B	345	GLY	O-C-CA-N
4	B	345	GLY	OXT-C-CA-N

Continued on next page...

*Continued from previous page...*

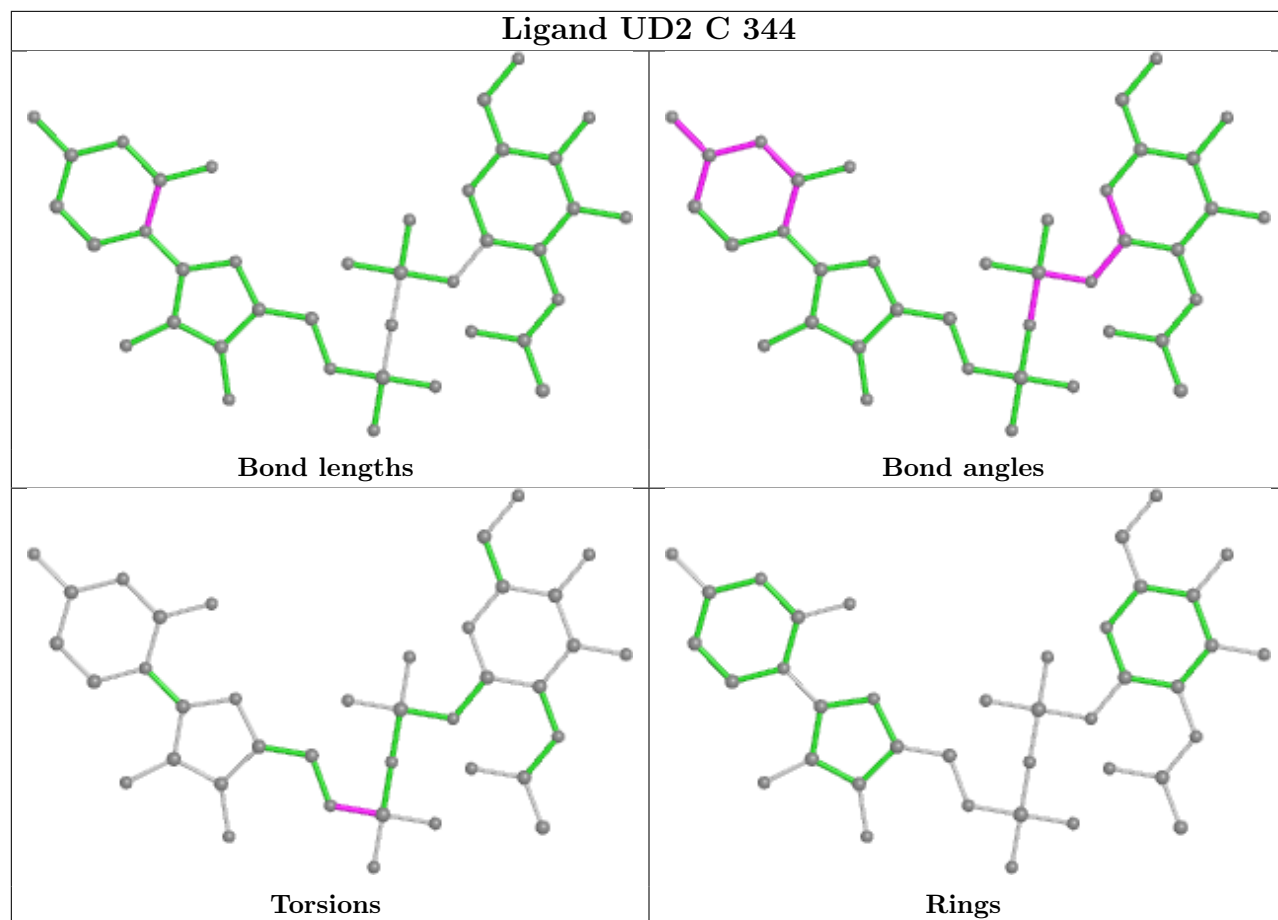
Mol	Chain	Res	Type	Atoms
2	B	343	NAD	O4B-C4B-C5B-O5B
3	D	343	UD2	C1'-O1'-PB-O3A
3	D	343	UD2	C3B-C4B-C5B-O5B
3	D	343	UD2	O4B-C4B-C5B-O5B
2	B	343	NAD	C3B-C4B-C5B-O5B
3	A	344	UD2	C4'-C5'-C6'-O6'
3	A	344	UD2	O5'-C5'-C6'-O6'
2	D	344	NAD	O4B-C4B-C5B-O5B
3	D	343	UD2	C1'-O1'-PB-O1B
2	A	343	NAD	PN-O3-PA-O5B
2	D	344	NAD	PN-O3-PA-O5B
2	C	343	NAD	O4B-C4B-C5B-O5B
2	D	344	NAD	C3B-C4B-C5B-O5B
3	D	343	UD2	C2B-C1B-N1-C6
2	A	343	NAD	C5B-O5B-PA-O3
2	B	343	NAD	C5B-O5B-PA-O3
2	C	343	NAD	C5B-O5B-PA-O3
2	D	344	NAD	C5B-O5B-PA-O3
3	C	344	UD2	C5B-O5B-PA-O3A
2	A	343	NAD	O4B-C4B-C5B-O5B
2	A	343	NAD	PA-O3-PN-O1N
2	A	343	NAD	C5B-O5B-PA-O1A
2	A	343	NAD	C5D-O5D-PN-O2N
2	B	343	NAD	C5B-O5B-PA-O1A
2	B	343	NAD	C5D-O5D-PN-O2N
2	C	343	NAD	C5B-O5B-PA-O1A
2	D	344	NAD	C5B-O5B-PA-O1A
3	A	344	UD2	O5'-C1'-O1'-PB
3	B	344	UD2	C1'-O1'-PB-O1B
3	D	343	UD2	O4B-C1B-N1-C6
3	B	344	UD2	C1'-O1'-PB-O3A
2	C	343	NAD	C3B-C4B-C5B-O5B
3	D	343	UD2	O4B-C1B-N1-C2
2	A	343	NAD	C3B-C4B-C5B-O5B
3	A	344	UD2	C3B-C4B-C5B-O5B
2	A	343	NAD	C5D-O5D-PN-O3
2	B	343	NAD	C5D-O5D-PN-O3
3	D	343	UD2	C5B-O5B-PA-O3A
3	D	343	UD2	C2B-C1B-N1-C2
2	B	343	NAD	PA-O3-PN-O1N

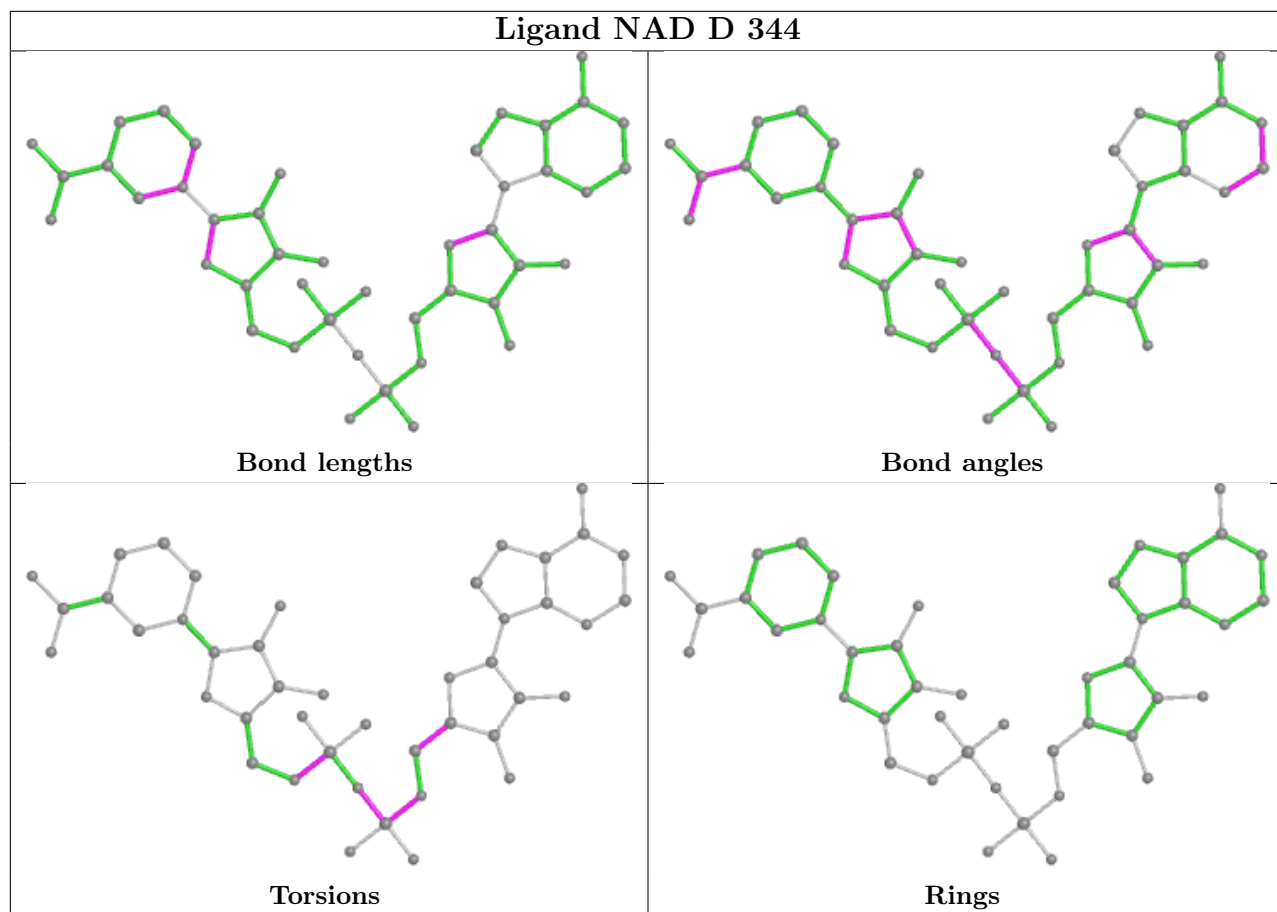
There are no ring outliers.

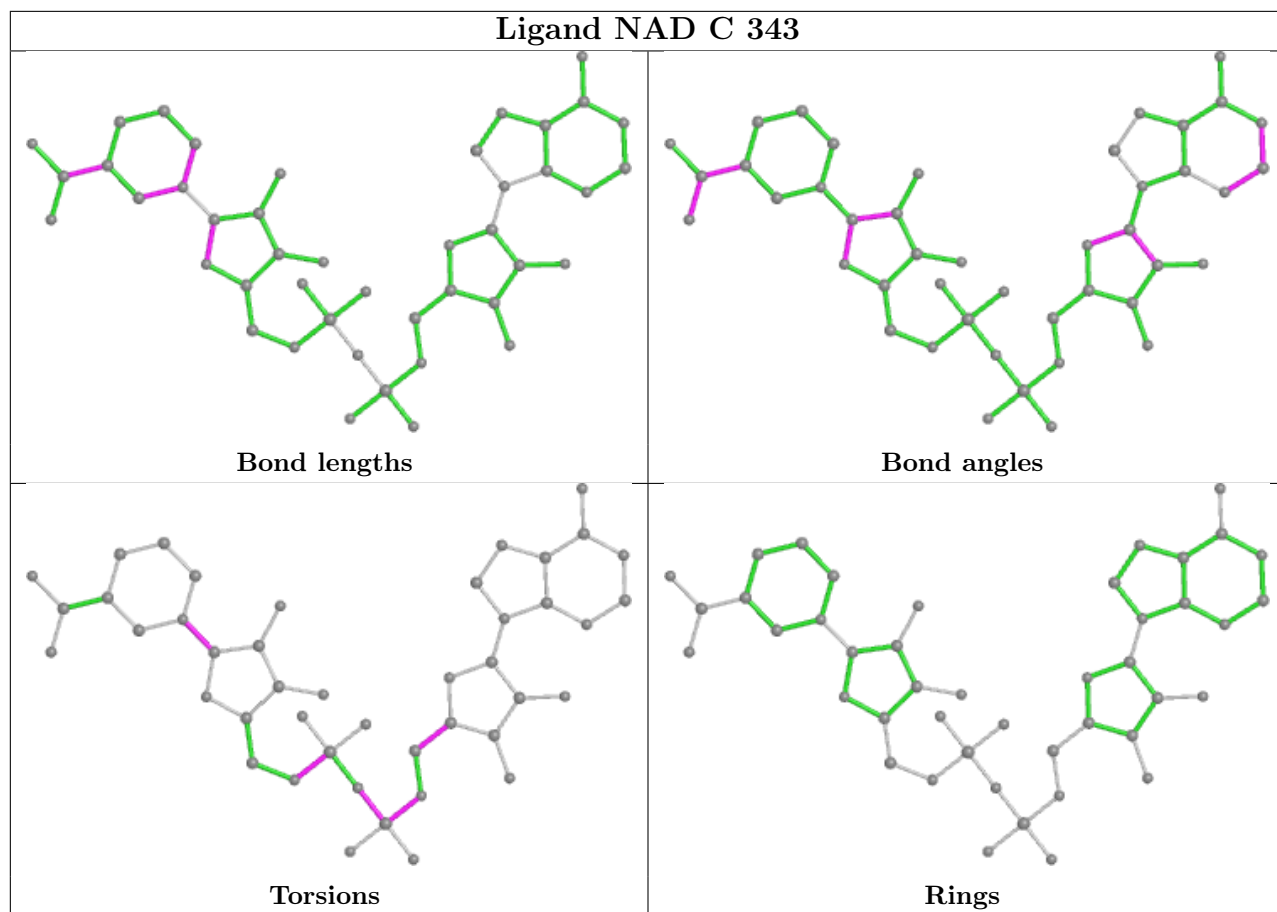
8 monomers are involved in 18 short contacts:

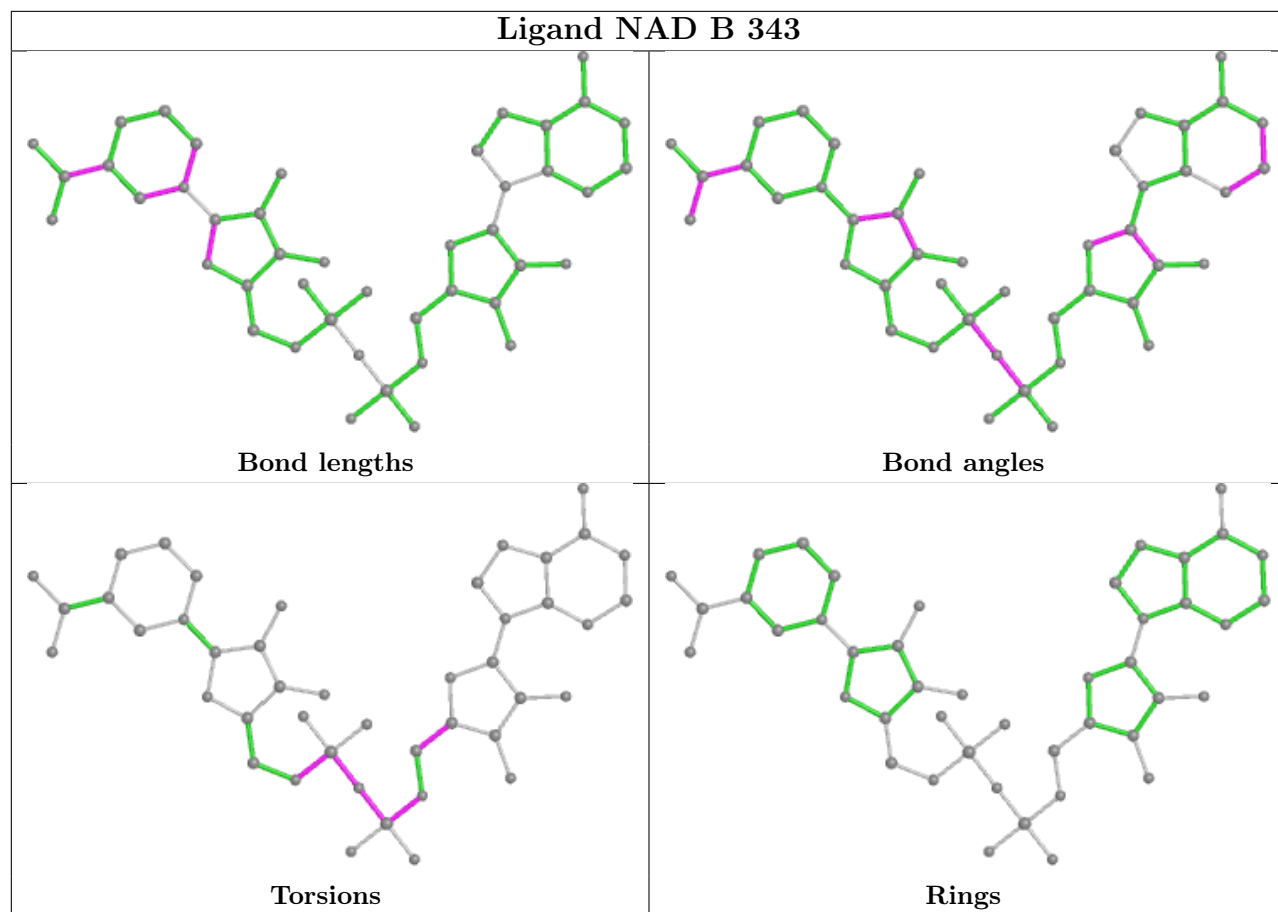
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	344	UD2	1	0
2	D	344	NAD	5	0
2	C	343	NAD	2	0
2	B	343	NAD	4	0
3	D	343	UD2	5	0
3	A	344	UD2	3	0
2	A	343	NAD	3	0
3	B	344	UD2	4	0

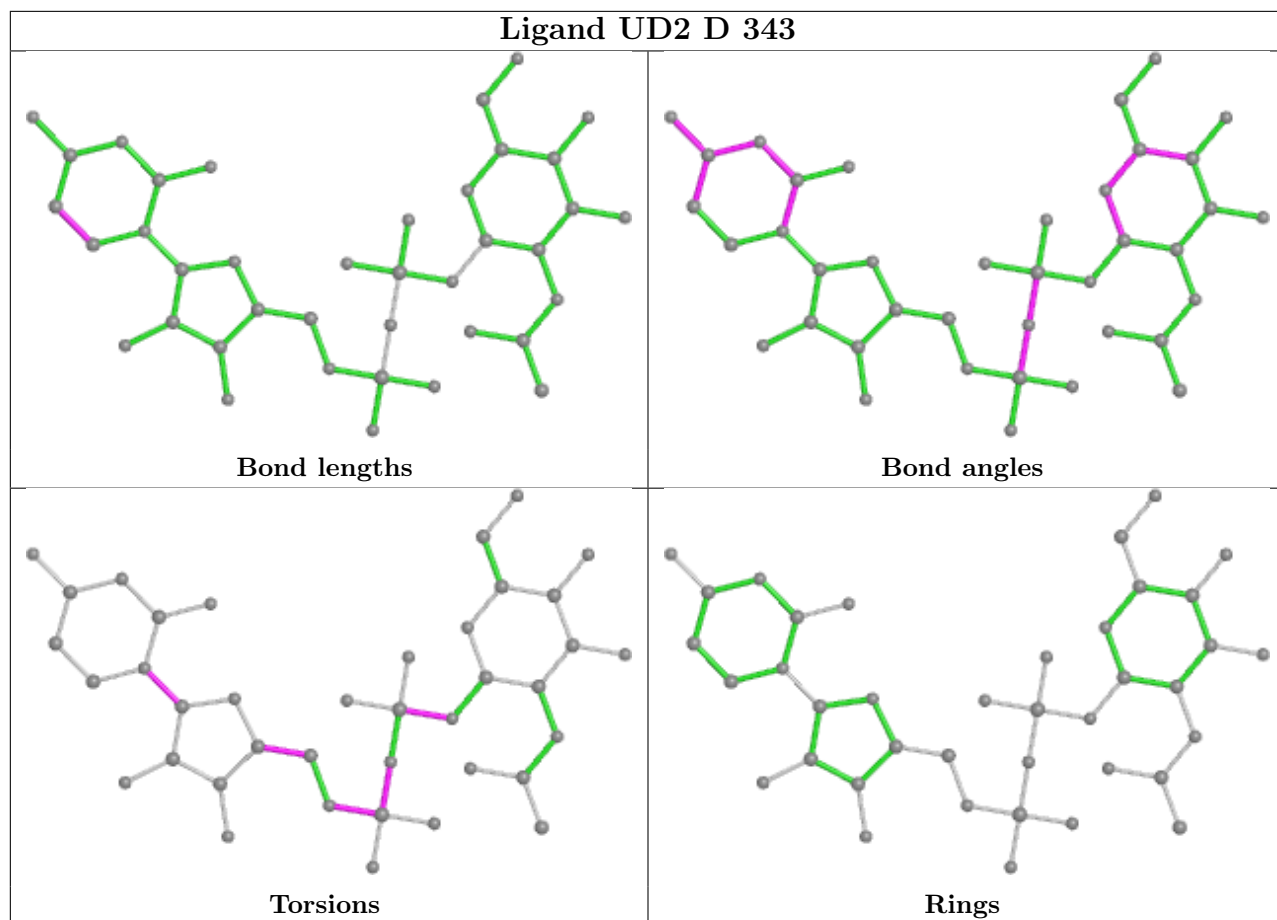
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



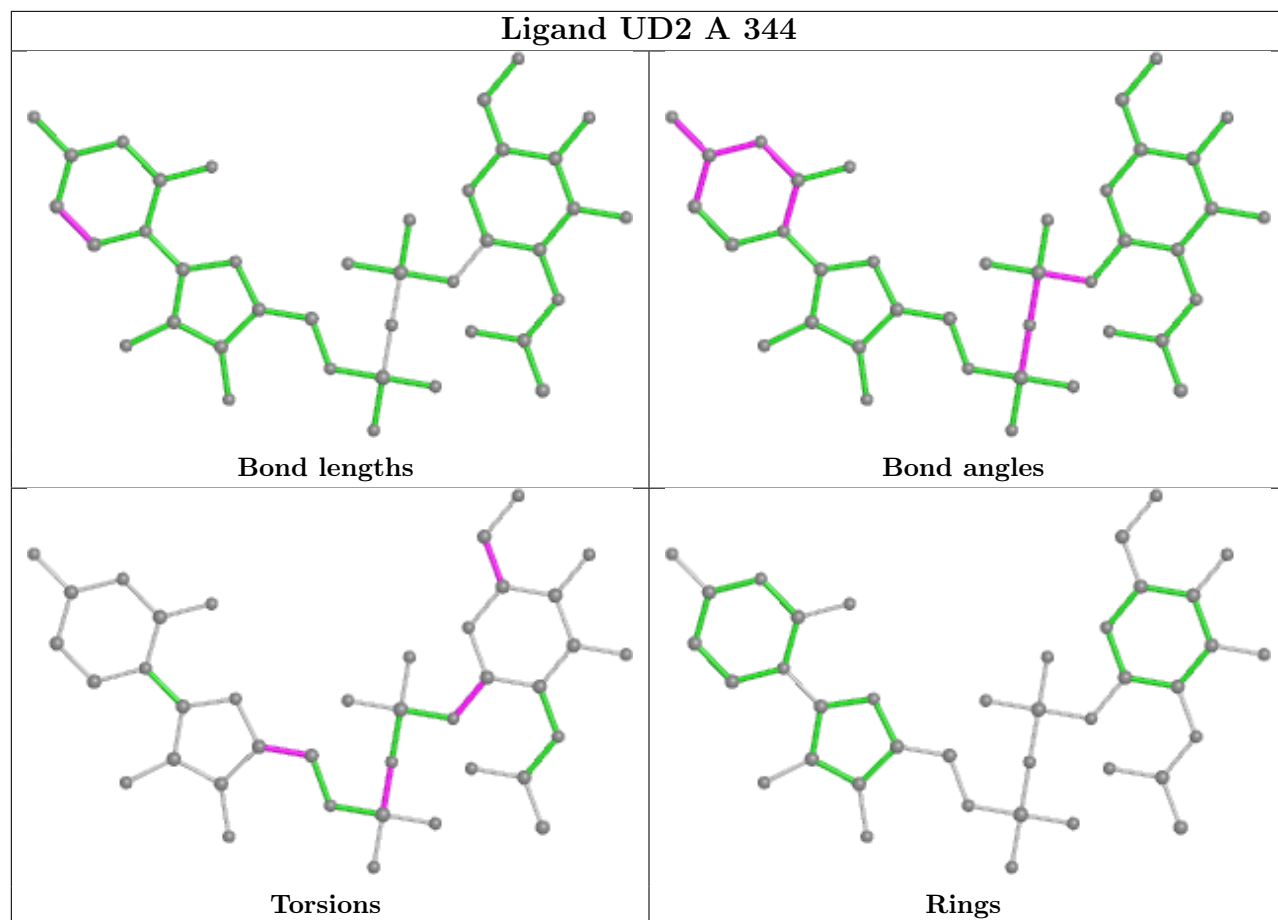


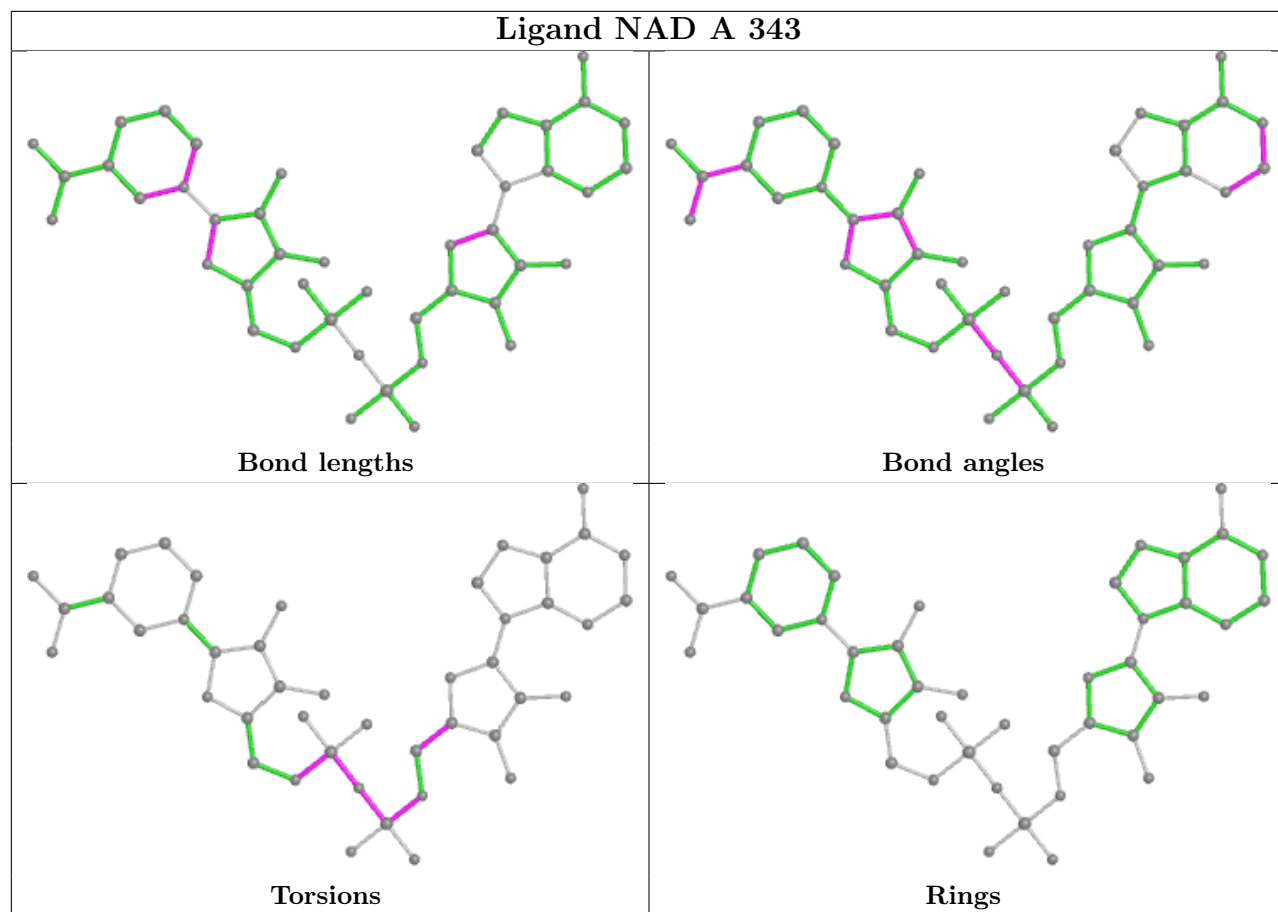


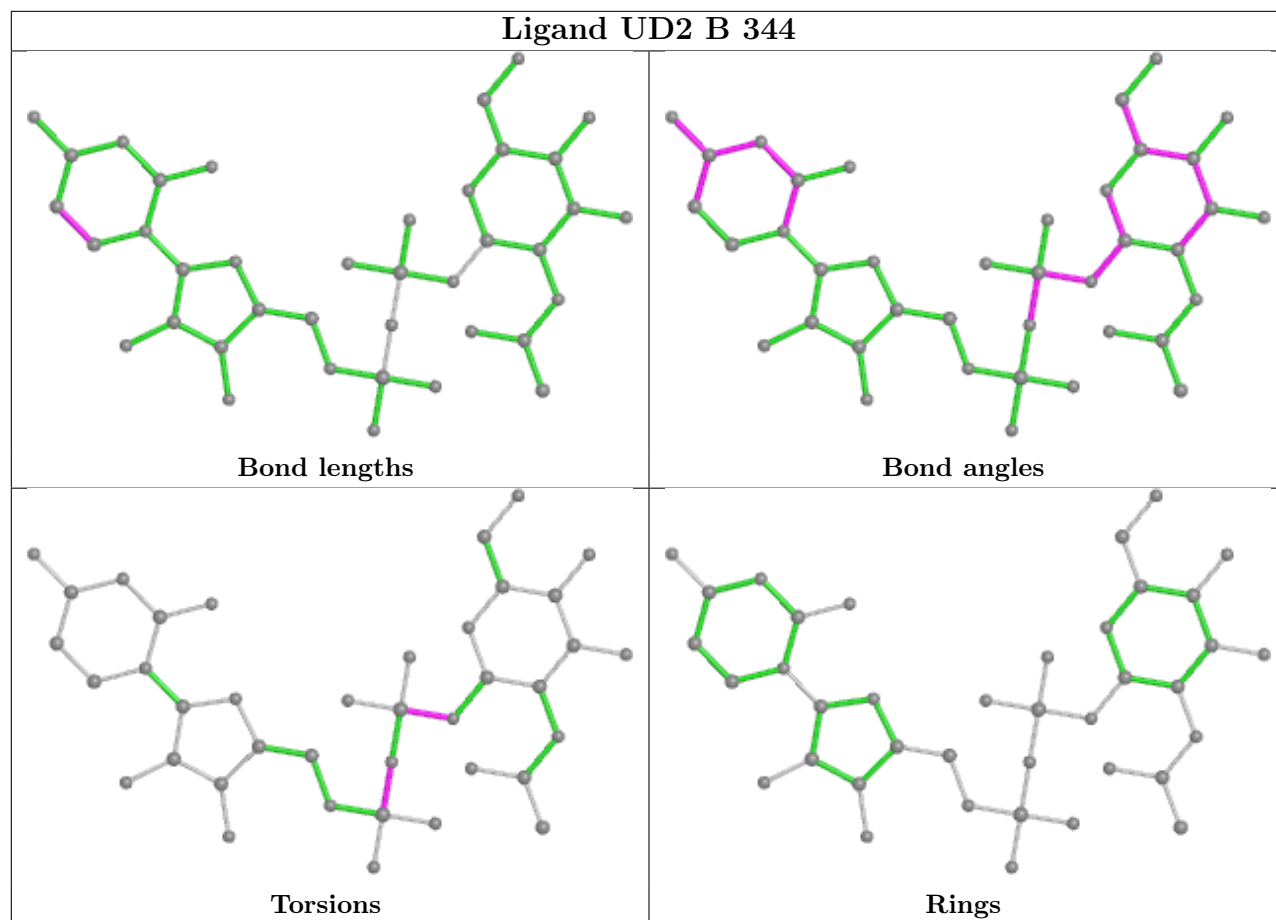












## 5.7 Other polymers [i](#)

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, 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	336/364 (92%)	-0.25	3 (0%) 84 86	24, 35, 59, 70	0
1	B	334/364 (91%)	-0.27	1 (0%) 94 94	25, 34, 50, 69	0
1	C	334/364 (91%)	-0.23	1 (0%) 94 94	23, 34, 51, 68	0
1	D	336/364 (92%)	-0.22	1 (0%) 94 94	23, 35, 60, 68	0
All	All	1340/1456 (92%)	-0.24	6 (0%) 92 93	23, 34, 56, 70	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	286	HIS	7.5
1	C	286	HIS	6.8
1	D	286	HIS	2.6
1	A	286	HIS	2.4
1	A	279	TYR	2.3
1	A	293	ILE	2.1

### 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,

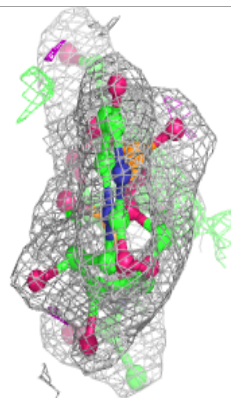
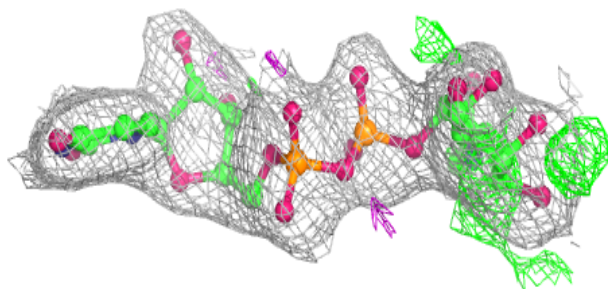
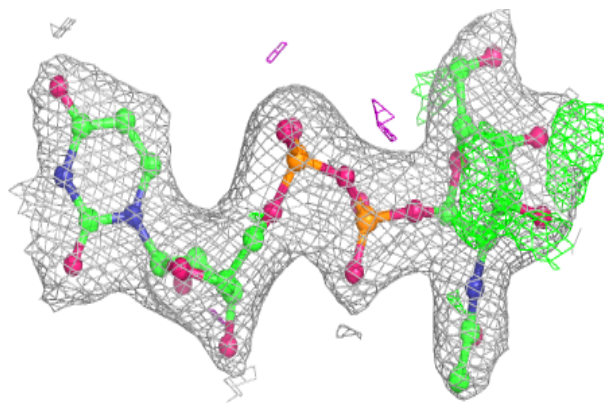
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GLY	B	345	5/5	0.88	0.18	68,68,68,68	0
3	UD2	D	343	39/39	0.93	0.15	31,37,44,45	14
3	UD2	A	344	39/39	0.94	0.15	31,40,46,46	14
3	UD2	C	344	39/39	0.94	0.13	18,28,33,34	14
4	GLY	D	348	5/5	0.94	0.12	52,53,53,53	0
6	NA	D	345	1/1	0.95	0.18	38,38,38,38	0
4	GLY	C	346	5/5	0.96	0.18	47,47,47,47	0
4	GLY	A	345	5/5	0.96	0.13	39,39,39,39	0
3	UD2	B	344	39/39	0.96	0.14	15,26,30,30	14
2	NAD	A	343	44/44	0.97	0.12	20,28,38,39	0
2	NAD	B	343	44/44	0.97	0.13	24,30,47,47	0
2	NAD	D	344	44/44	0.97	0.12	18,26,41,43	0
5	SO4	C	345	5/5	0.98	0.10	47,47,47,48	0
5	SO4	D	346	5/5	0.98	0.12	44,44,45,45	0
5	SO4	D	347	5/5	0.98	0.12	41,41,43,43	0
2	NAD	C	343	44/44	0.98	0.12	25,30,45,45	0

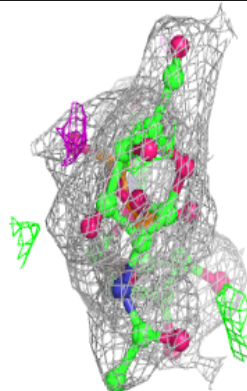
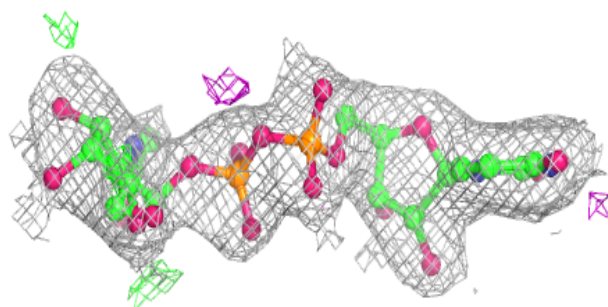
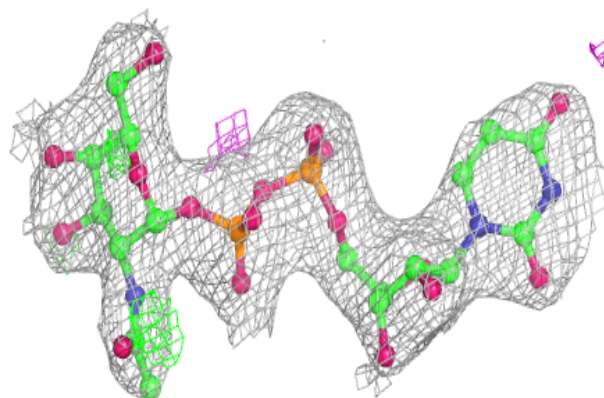
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around UD2 D 343:**

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

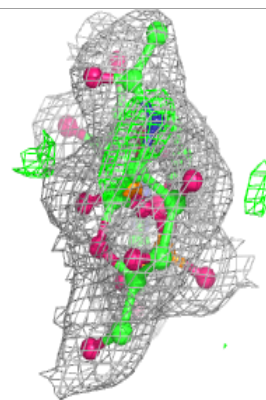
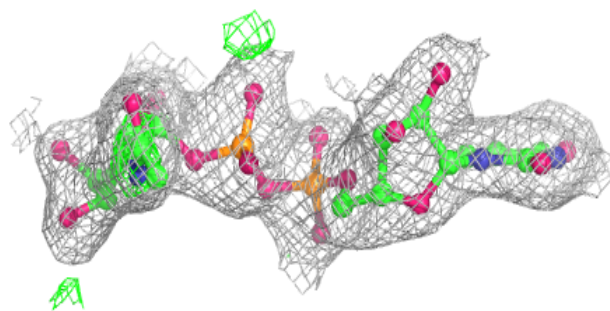
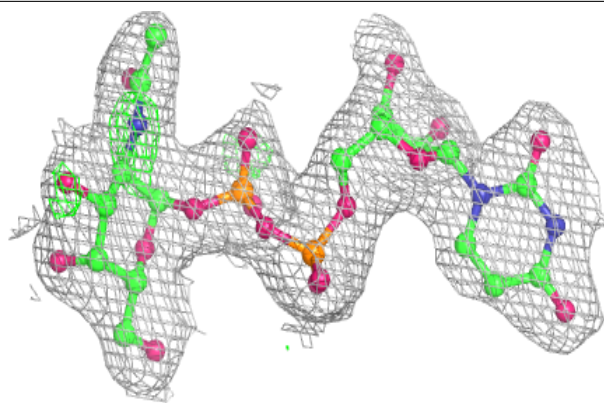
**Electron density around UD2 A 344:**

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

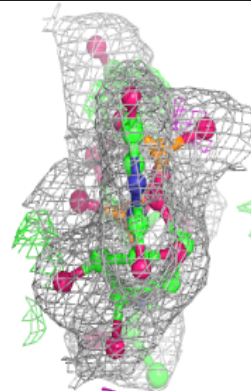
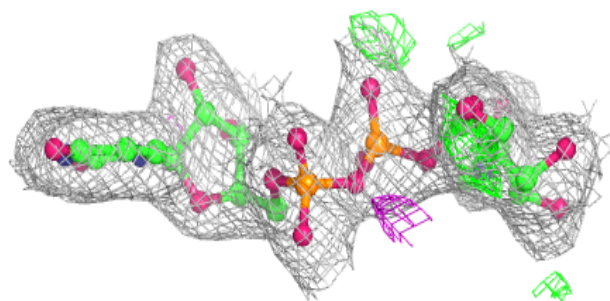
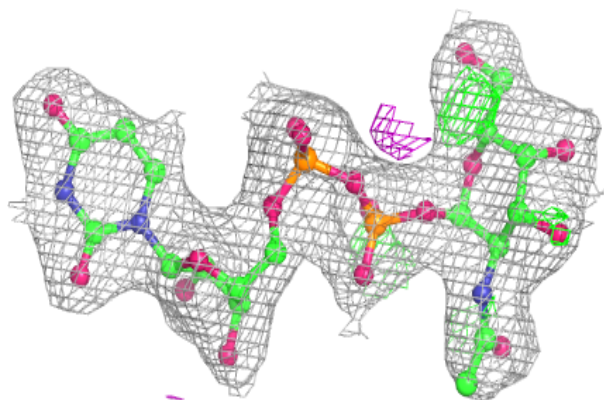


**Electron density around UD2 C 344:**

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

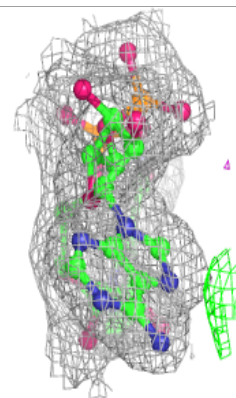
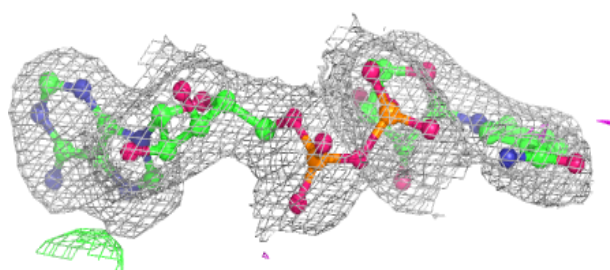
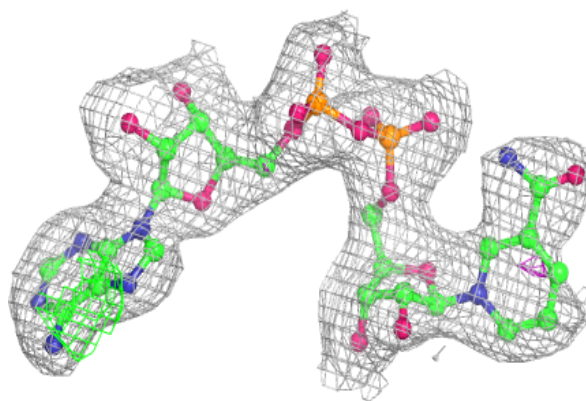
**Electron density around UD2 B 344:**

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

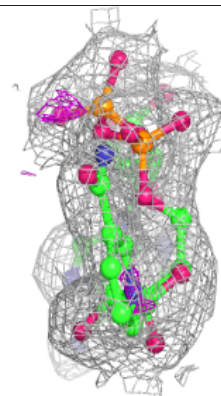
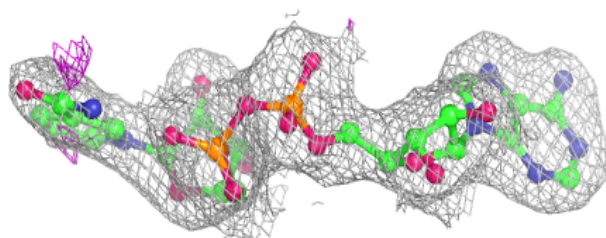
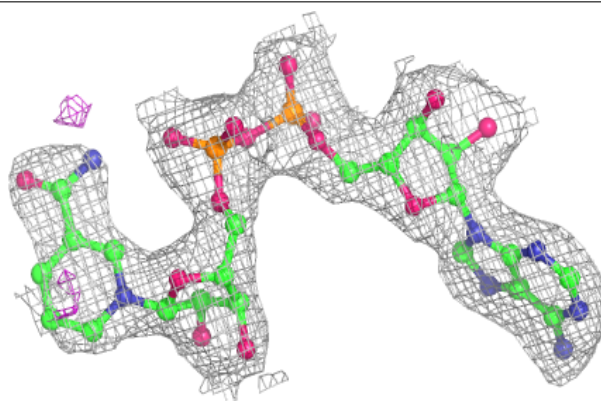


**Electron density around NAD A 343:**

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

**Electron density around NAD B 343:**

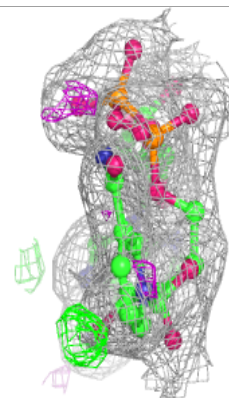
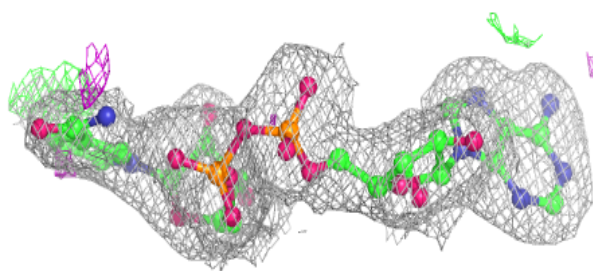
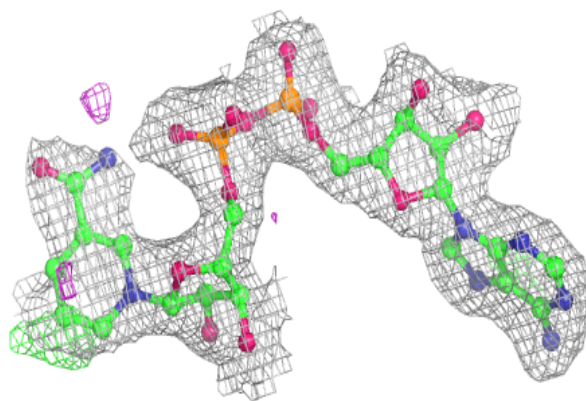
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



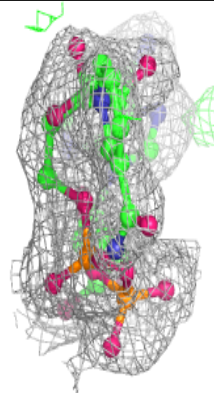
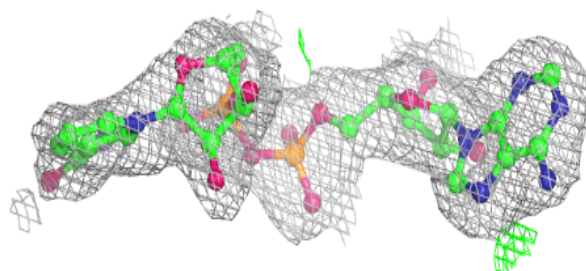
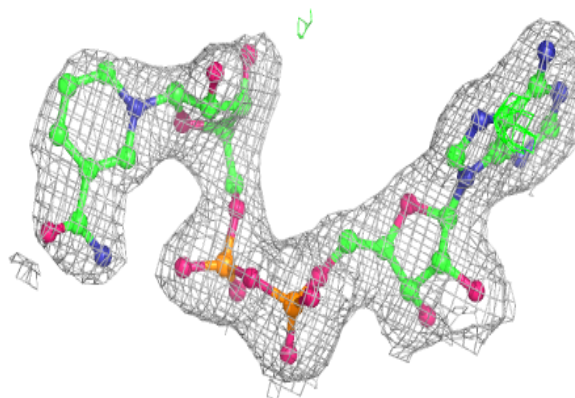


**Electron density around NAD D 344:**

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

**Electron density around NAD C 343:**

$2mF_o-DF_c$  (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.