



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:29 pm BST

PDB ID : 3RUH  
Title : Alternative analogs as viable substrates of UDP-hexose 4-epimerases  
Authors : Bhatt, V.S.; Guan, W.; Wang, P.G.  
Deposited on : 2011-05-05  
Resolution : 2.88 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.

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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 : 2.11  
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) : 2.11

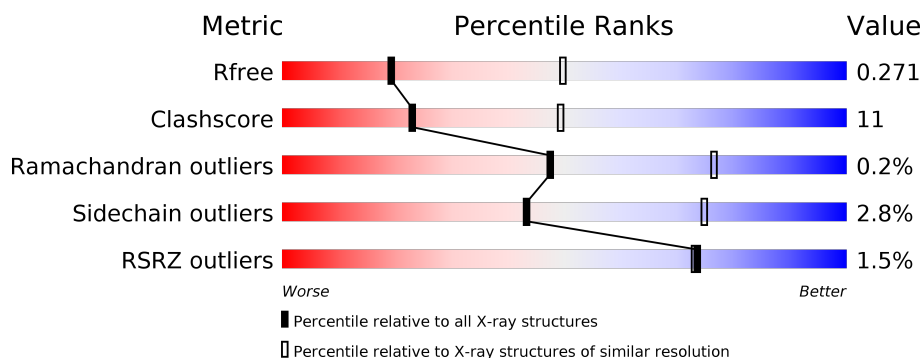
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.88 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 on 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	351	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• •</div> </div> </div>
1	B	351	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>
1	C	351	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
1	D	351	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11113 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
1	A	336	Total	C	N	O	S	0	0	0
			2681	1712	459	502	8			
1	B	336	Total	C	N	O	S	0	0	0
			2681	1712	459	502	8			
1	C	336	Total	C	N	O	S	0	0	0
			2681	1712	459	502	8			
1	D	336	Total	C	N	O	S	0	0	0
			2681	1712	459	502	8			

There are 24 discrepancies between the modelled and reference sequences:

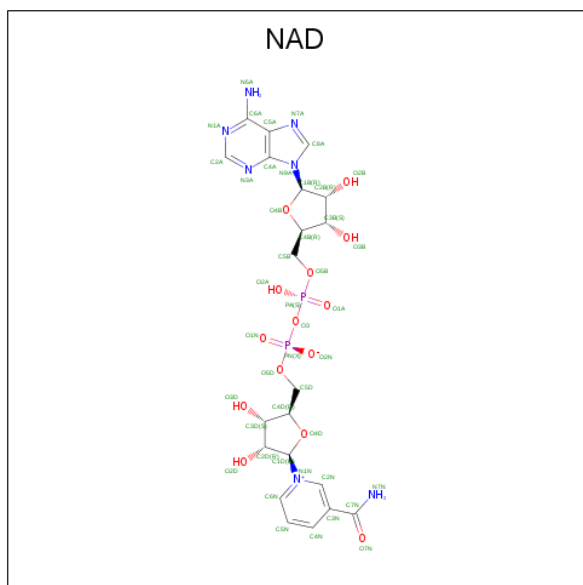
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
B	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
C	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9

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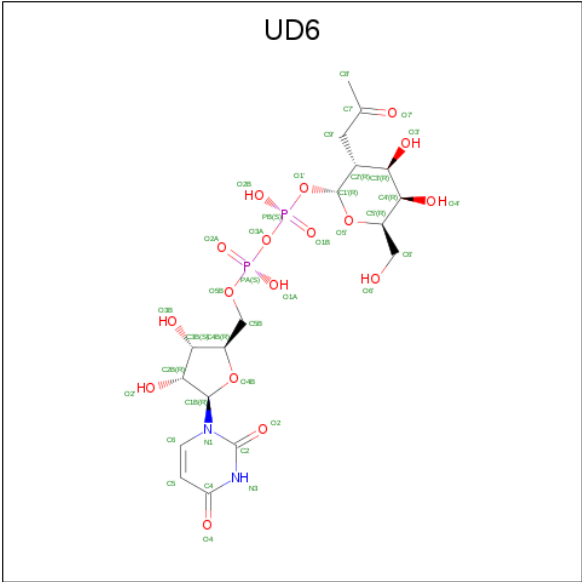
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9

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



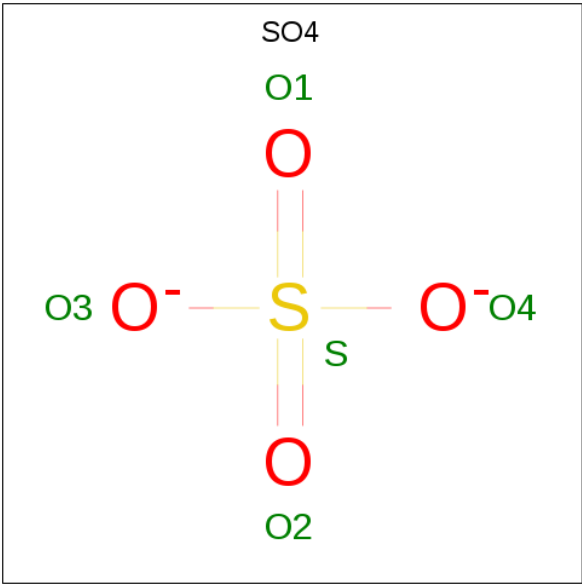
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is [(2R,3S,4R,5R)-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl [(2R,3R,4R,5R,6R)-6-(hydroxymethyl)-4,5-bis(oxidanyl)-3-(2-oxidanylidenepropyl)oxan-2-yl] hydrogen phosphate (three-letter code: UD6) (formula: C<sub>18</sub>H<sub>28</sub>N<sub>2</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			39	18	2	17	2		
3	B	1	Total	C	N	O	P	0	0
			39	18	2	17	2		
3	C	1	Total	C	N	O	P	0	0
			39	18	2	17	2		
3	D	1	Total	C	N	O	P	0	0
			39	18	2	17	2		

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



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0

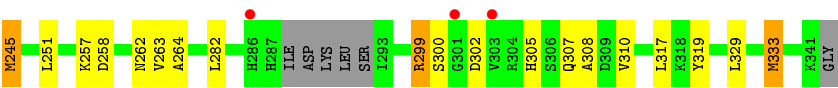
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0
6	B	10	Total O 10 10	0	0
6	C	13	Total O 13 13	0	0
6	D	11	Total O 11 11	0	0

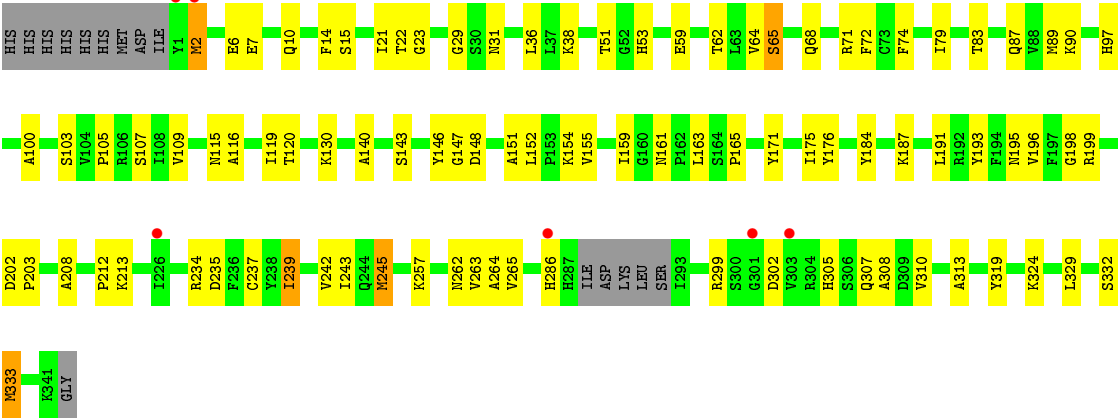


- Molecule 1: WbgU





● Molecule 1: WbgU





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.61Å 76.61Å 220.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	73.53 – 2.88 30.24 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.2 (73.53-2.88) 98.3 (30.24-2.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.210 , 0.268 0.210 , 0.271	Depositor DCC
$R_{free}$ test set	1632 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 4.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l 0.457 for h,-h-k,-l 0.050 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, UD6, SO4, 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	0.49	5/2739 (0.2%)	0.55	0/3717
1	B	0.48	4/2739 (0.1%)	0.55	0/3717
1	C	0.48	3/2739 (0.1%)	0.56	0/3717
1	D	0.48	2/2739 (0.1%)	0.56	0/3717
All	All	0.48	14/10956 (0.1%)	0.56	0/14868

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	2	MET	CG-SD	8.12	2.02	1.81
1	C	2	MET	CG-SD	7.84	2.01	1.81
1	A	333	MET	CG-SD	6.05	1.96	1.81
1	B	333	MET	CG-SD	5.91	1.96	1.81
1	A	2	MET	CG-SD	5.58	1.95	1.81
1	B	2	MET	CG-SD	5.45	1.95	1.81
1	C	333	MET	CG-SD	5.43	1.95	1.81
1	D	333	MET	CG-SD	5.33	1.95	1.81
1	A	245	MET	CG-SD	5.27	1.94	1.81
1	A	89	MET	CG-SD	5.21	1.94	1.81
1	B	245	MET	CG-SD	5.14	1.94	1.81
1	A	218	MET	CG-SD	5.12	1.94	1.81
1	B	218	MET	CG-SD	5.08	1.94	1.81
1	C	245	MET	CG-SD	5.06	1.94	1.81

There are no bond angle outliers.

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	2681	0	2658	64	0
1	B	2681	0	2658	64	0
1	C	2681	0	2658	56	0
1	D	2681	0	2658	59	0
2	A	44	0	26	11	0
2	B	44	0	26	5	0
2	C	44	0	26	8	0
2	D	44	0	26	6	0
3	A	39	0	26	4	0
3	B	39	0	26	4	0
3	C	39	0	26	5	0
3	D	39	0	26	5	0
4	A	15	0	0	0	0
5	A	1	0	0	0	0
6	A	7	0	0	1	0
6	B	10	0	0	0	0
6	C	13	0	0	1	0
6	D	11	0	0	0	0
All	All	11113	0	10840	250	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 11.

All (250) 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:2:MET:SD	1:C:2:MET:CG	2.01	1.49
1:D:2:MET:CG	1:D:2:MET:SD	2.02	1.47
2:A:343:NAD:C4N	3:A:344:UD6:H4'	1.80	1.11
2:C:343:NAD:C4N	3:C:344:UD6:H4'	1.88	1.03
1:D:245:MET:HG2	1:D:263:VAL:HG22	1.47	0.95
1:C:245:MET:HG2	1:C:263:VAL:HG22	1.48	0.93
1:A:245:MET:HG2	1:A:263:VAL:HG22	1.49	0.92
1:B:245:MET:HG2	1:B:263:VAL:HG22	1.52	0.89
2:A:343:NAD:H2N	2:A:343:NAD:H52N	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:343:NAD:H4N	3:A:344:UD6:H4'	1.55	0.88
1:C:299:ARG:HB3	1:C:302:ASP:HB2	1.55	0.88
1:B:71:ARG:HH11	1:B:71:ARG:HG2	1.38	0.87
1:B:6:GLU:O	1:B:10:GLN:HG2	1.78	0.82
2:D:343:NAD:C4N	3:D:344:UD6:H4'	2.09	0.82
1:A:14:PHE:CZ	1:B:105:PRO:HB3	2.15	0.81
1:B:21:ILE:HD11	1:B:36:LEU:HD12	1.64	0.78
1:A:148:ASP:HB3	1:A:163:LEU:HD21	1.66	0.77
2:A:343:NAD:H2N	2:A:343:NAD:C5D	2.14	0.77
2:B:343:NAD:C4N	3:B:344:UD6:H4'	2.19	0.72
1:D:116:ALA:O	1:D:120:THR:HB	1.90	0.71
1:D:299:ARG:HB3	1:D:302:ASP:HB2	1.71	0.71
2:C:343:NAD:H4N	3:C:344:UD6:H4'	1.74	0.69
1:A:102:GLY:O	1:A:103:SER:HB3	1.90	0.69
1:B:117:THR:HG23	2:B:343:NAD:H61A	1.58	0.69
1:B:8:ILE:HD12	1:B:248:LEU:HD23	1.74	0.69
1:D:53:HIS:NE2	1:D:202:ASP:OD2	2.26	0.68
1:A:264:ALA:HB3	1:A:308:ALA:HB3	1.75	0.68
1:A:304:ARG:HG3	1:A:305:HIS:CD2	2.29	0.67
1:A:245:MET:CE	1:A:313:ALA:CB	2.73	0.66
1:A:12:LEU:HD21	1:A:251:LEU:HD11	1.75	0.66
1:D:21:ILE:HD11	1:D:36:LEU:HD12	1.77	0.66
1:A:71:ARG:HH11	1:A:71:ARG:HG2	1.58	0.66
1:D:245:MET:CG	1:D:263:VAL:HG22	2.26	0.66
1:C:21:ILE:HD11	1:C:36:LEU:HD12	1.77	0.65
1:D:107:SER:HB2	1:D:165:PRO:HB2	1.78	0.65
1:B:148:ASP:HB3	1:B:163:LEU:HD21	1.78	0.65
1:B:203:PRO:HA	1:B:212:PRO:HB2	1.80	0.64
1:B:71:ARG:HH11	1:B:71:ARG:CG	2.10	0.64
1:B:102:GLY:O	1:B:103:SER:HB3	1.96	0.64
1:A:117:THR:HG23	2:A:343:NAD:H61A	1.62	0.63
1:A:116:ALA:O	1:A:120:THR:HB	1.98	0.63
1:A:245:MET:CE	1:A:313:ALA:HB1	2.29	0.62
1:B:195:ASN:OD1	1:B:234:ARG:HG3	2.00	0.62
1:D:203:PRO:HA	1:D:212:PRO:HB2	1.81	0.62
1:C:103:SER:OG	1:C:105:PRO:HD2	2.00	0.61
1:A:245:MET:HE1	1:A:313:ALA:CB	2.31	0.60
1:C:117:THR:HG23	2:C:343:NAD:H61A	1.65	0.60
1:C:203:PRO:HA	1:C:212:PRO:HB2	1.84	0.60
1:C:152:LEU:HD11	1:C:305:HIS:HB3	1.84	0.60
1:C:107:SER:HB2	1:C:165:PRO:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ALA:O	1:C:120:THR:HB	2.01	0.59
1:D:235:ASP:HB2	1:D:307:GLN:HA	1.84	0.59
1:A:245:MET:HE3	1:A:313:ALA:CB	2.33	0.59
1:C:310:VAL:HG11	1:C:319:TYR:HE2	1.67	0.59
1:C:50:SER:HB2	1:D:14:PHE:CG	2.38	0.59
1:D:65:SER:HB3	1:D:68:GLN:HG3	1.85	0.59
1:B:304:ARG:HG3	1:B:305:HIS:CD2	2.38	0.58
1:C:171:TYR:CZ	1:C:175:ILE:HD11	2.38	0.58
1:D:171:TYR:CZ	1:D:175:ILE:HD11	2.39	0.58
1:B:245:MET:HG2	1:B:263:VAL:CG2	2.27	0.58
1:A:71:ARG:HH11	1:A:71:ARG:CG	2.17	0.58
1:B:105:PRO:HG2	1:B:299:ARG:HH11	1.69	0.58
1:A:8:ILE:HD12	1:A:248:LEU:HD23	1.86	0.57
1:D:191:LEU:HD22	1:D:245:MET:HG3	1.86	0.57
1:A:245:MET:HE3	1:A:313:ALA:HB2	1.87	0.56
1:C:106:ARG:NH1	1:D:14:PHE:O	2.31	0.56
1:A:6:GLU:O	1:A:10:GLN:HG2	2.03	0.56
1:B:102:GLY:HA2	1:B:166:TYR:CE1	2.40	0.56
1:B:233:SER:HB2	1:B:268:ARG:HG2	1.87	0.56
1:A:102:GLY:HA2	1:A:166:TYR:CE1	2.41	0.56
1:A:203:PRO:HA	1:A:212:PRO:HB2	1.88	0.56
1:B:177:ALA:HB1	1:B:188:THR:OG1	2.05	0.56
1:C:31:ASN:HB3	1:C:243:ILE:HD11	1.88	0.55
1:B:227:ASN:HD21	1:B:299:ARG:HH21	1.52	0.55
1:A:5:TYR:CG	1:A:244:GLN:HG3	2.41	0.55
2:D:343:NAD:H4N	3:D:344:UD6:H4'	1.85	0.55
1:D:148:ASP:HB3	1:D:163:LEU:HD21	1.88	0.55
2:A:343:NAD:H52N	2:A:343:NAD:C2N	2.32	0.55
1:A:245:MET:CE	1:A:313:ALA:HB2	2.37	0.54
1:B:171:TYR:CE2	1:B:175:ILE:HD11	2.42	0.54
1:B:338:ARG:HB2	1:B:338:ARG:HH11	1.73	0.54
1:C:147:GLY:HA3	1:C:161:ASN:O	2.07	0.54
1:C:310:VAL:O	1:C:310:VAL:HG12	2.07	0.53
1:C:207:TYR:HE1	1:D:71:ARG:NH2	2.07	0.53
1:A:105:PRO:HG2	1:A:299:ARG:NH1	2.23	0.53
1:A:197:PHE:HA	1:A:201:GLN:OE1	2.09	0.53
1:C:329:LEU:O	1:C:333:MET:HG2	2.08	0.53
1:D:143:SER:OG	3:D:344:UD6:H9'A	2.08	0.53
1:B:233:SER:HA	1:B:270:THR:HA	1.90	0.52
1:B:116:ALA:O	1:B:120:THR:HB	2.08	0.52
1:A:16:PRO:HA	1:A:41:GLN:HE22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:PRO:HG2	1:A:299:ARG:HH11	1.74	0.52
1:D:31:ASN:HB3	1:D:243:ILE:HD11	1.91	0.52
1:C:310:VAL:CG1	1:C:310:VAL:O	2.57	0.52
1:D:147:GLY:HA3	1:D:161:ASN:O	2.10	0.52
1:C:114:THR:HG22	1:C:169:THR:HG21	1.90	0.52
1:D:310:VAL:HG12	1:D:310:VAL:O	2.09	0.52
1:A:264:ALA:HB3	1:A:308:ALA:CB	2.40	0.52
1:D:152:LEU:HD11	1:D:305:HIS:HB3	1.90	0.52
1:D:310:VAL:HG11	1:D:319:TYR:CE2	2.45	0.51
1:C:148:ASP:HB3	1:C:163:LEU:HD21	1.92	0.51
1:B:147:GLY:HA3	1:B:161:ASN:O	2.11	0.51
1:A:33:LEU:HD23	1:A:60:VAL:HG11	1.93	0.51
1:C:53:HIS:NE2	1:C:202:ASP:OD2	2.43	0.51
1:B:71:ARG:CG	1:B:71:ARG:NH1	2.73	0.50
1:A:137:PHE:HB3	1:A:188:THR:HG22	1.93	0.50
1:D:103:SER:OG	1:D:105:PRO:HD2	2.11	0.50
1:D:310:VAL:HG11	1:D:319:TYR:HE2	1.76	0.50
1:C:215:THR:HG23	1:C:282:LEU:HD11	1.93	0.50
1:C:170:LYS:HE3	2:C:343:NAD:O2D	2.11	0.50
1:B:168:VAL:CG2	1:C:179:VAL:HG21	2.42	0.49
1:C:154:LYS:O	1:C:262:ASN:ND2	2.44	0.49
1:A:168:VAL:O	1:A:172:VAL:HG23	2.12	0.49
1:C:187:LYS:HG2	1:C:258:ASP:HB2	1.94	0.49
1:A:117:THR:HG23	2:A:343:NAD:N6A	2.28	0.49
2:C:343:NAD:C4N	3:C:344:UD6:C4'	2.76	0.49
2:C:343:NAD:C5N	3:C:344:UD6:H4'	2.41	0.49
1:A:245:MET:HG2	1:A:263:VAL:CG2	2.32	0.49
1:A:233:SER:HA	1:A:270:THR:HA	1.95	0.49
1:D:187:LYS:HB3	1:D:257:LYS:HB3	1.95	0.49
1:C:149:HIS:HD2	1:C:151:ALA:H	1.58	0.49
1:D:245:MET:CE	1:D:313:ALA:HB1	2.42	0.49
1:A:59:GLU:O	1:A:62:THR:HB	2.12	0.48
1:C:78:ASP:OD2	1:C:80:ARG:NH2	2.44	0.48
1:D:329:LEU:O	1:D:333:MET:HG2	2.12	0.48
1:B:123:LEU:HG	1:C:112:ILE:HD13	1.94	0.48
1:C:300:SER:HB2	6:C:356:HOH:O	2.14	0.48
1:A:233:SER:OG	1:A:305:HIS:ND1	2.41	0.48
1:B:78:ASP:OD1	2:B:343:NAD:N6A	2.46	0.48
1:D:265:VAL:HG11	1:D:324:LYS:HG3	1.96	0.48
1:A:53:HIS:NE2	1:A:202:ASP:OD2	2.44	0.48
1:D:198:GLY:HA2	1:D:332:SER:OG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TYR:CE2	1:A:175:ILE:HD11	2.47	0.48
1:B:168:VAL:O	1:B:172:VAL:HG23	2.14	0.48
1:B:234:ARG:NH2	3:B:344:UD6:H8'B	2.29	0.48
1:A:239:ILE:HG13	1:A:239:ILE:H	1.43	0.47
1:B:105:PRO:HG2	1:B:299:ARG:NH1	2.28	0.47
1:B:107:SER:HB2	1:B:165:PRO:HB2	1.96	0.47
1:A:193:TYR:HB2	2:A:343:NAD:C5N	2.44	0.47
1:D:196:VAL:HA	1:D:237:CYS:O	2.13	0.47
1:D:208:ALA:HB3	1:D:213:LYS:HD3	1.96	0.47
1:A:105:PRO:CG	1:A:299:ARG:HH11	2.26	0.47
1:D:195:ASN:OD1	1:D:234:ARG:HG3	2.15	0.47
1:A:177:ALA:HB1	1:A:188:THR:OG1	2.15	0.47
1:A:338:ARG:HB2	1:A:338:ARG:HH11	1.79	0.47
1:C:193:TYR:HB2	2:C:343:NAD:C5N	2.44	0.47
1:D:130:LYS:HD2	1:D:184:TYR:CG	2.49	0.47
1:B:100:ALA:HB3	2:B:343:NAD:O3D	2.15	0.47
1:D:151:ALA:O	1:D:154:LYS:HD3	2.13	0.47
1:D:65:SER:CB	1:D:68:GLN:HG3	2.44	0.47
1:B:229:ASP:OD2	1:B:231:GLU:HB2	2.15	0.47
1:D:310:VAL:O	1:D:310:VAL:CG1	2.63	0.46
1:B:59:GLU:O	1:B:62:THR:HB	2.15	0.46
1:C:109:VAL:HG21	1:D:71:ARG:HD2	1.98	0.46
1:D:154:LYS:O	1:D:262:ASN:ND2	2.48	0.46
1:B:102:GLY:O	1:B:103:SER:CB	2.60	0.46
1:A:245:MET:HE1	1:A:313:ALA:HB1	1.95	0.46
1:C:168:VAL:O	1:C:172:VAL:HG23	2.16	0.46
2:A:343:NAD:C5N	3:A:344:UD6:H4'	2.42	0.46
1:A:107:SER:HB2	1:A:165:PRO:HB2	1.97	0.45
1:B:264:ALA:HB3	1:B:308:ALA:HB3	1.97	0.45
1:A:311:THR:HA	1:A:314:ILE:HD12	1.98	0.45
1:D:264:ALA:HB3	1:D:308:ALA:HB3	1.97	0.45
1:A:304:ARG:HG3	1:A:305:HIS:HD2	1.78	0.45
1:A:187:LYS:HB3	1:A:257:LYS:HB3	1.99	0.45
1:B:197:PHE:HA	1:B:201:GLN:OE1	2.16	0.45
1:C:5:TYR:CG	1:C:244:GLN:HG3	2.52	0.45
1:C:235:ASP:HB2	1:C:307:GLN:HA	1.99	0.45
1:D:23:GLY:O	1:D:29:GLY:HA3	2.17	0.45
1:D:245:MET:CE	1:D:313:ALA:CB	2.95	0.45
1:B:143:SER:OG	3:B:344:UD6:H9'A	2.17	0.45
1:D:245:MET:HE1	1:D:313:ALA:HB1	1.98	0.45
1:A:107:SER:HB3	1:A:166:TYR:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ALA:HB3	1:C:213:LYS:HD3	1.99	0.44
1:C:187:LYS:HB3	1:C:257:LYS:HB3	1.99	0.44
1:B:233:SER:OG	1:B:305:HIS:ND1	2.35	0.44
1:C:12:LEU:HD21	1:C:251:LEU:HD11	2.00	0.44
1:C:46:LEU:HD22	1:C:88:VAL:HG21	1.99	0.44
1:D:242:VAL:HG22	1:D:263:VAL:HG11	1.98	0.44
1:A:232:THR:CG2	1:A:234:ARG:NH1	2.80	0.44
1:B:33:LEU:HD23	1:B:60:VAL:HG11	1.99	0.44
1:C:245:MET:HE1	1:C:317:LEU:HD12	2.00	0.44
1:A:51:THR:OG1	2:A:343:NAD:H2B	2.17	0.44
1:B:12:LEU:HD21	1:B:251:LEU:HD11	1.98	0.44
1:D:100:ALA:HB3	2:D:343:NAD:H3D	2.00	0.44
2:D:343:NAD:H5N	3:D:344:UD6:O3'	2.18	0.44
1:A:71:ARG:CG	1:A:71:ARG:NH1	2.78	0.44
1:B:264:ALA:HB3	1:B:308:ALA:CB	2.48	0.43
1:B:5:TYR:CG	1:B:244:GLN:HG3	2.53	0.43
1:A:333:MET:HB2	1:A:334:PRO:HD3	1.99	0.43
1:C:10:GLN:O	1:C:14:PHE:HD2	2.01	0.43
1:C:264:ALA:HB3	1:C:308:ALA:HB3	2.00	0.43
1:C:310:VAL:HG11	1:C:319:TYR:CE2	2.50	0.43
1:B:107:SER:HB3	1:B:166:TYR:HB2	2.01	0.43
1:D:6:GLU:O	1:D:10:GLN:HG2	2.18	0.43
1:A:314:ILE:O	1:A:318:LYS:HA	2.18	0.43
1:B:179:VAL:HG21	1:C:168:VAL:HG23	2.00	0.43
2:A:343:NAD:C4N	3:A:344:UD6:C4'	2.73	0.43
1:A:5:TYR:CD2	1:A:244:GLN:HG3	2.54	0.43
1:B:193:TYR:HB2	2:B:343:NAD:C5N	2.49	0.43
1:B:103:SER:H	3:B:344:UD6:C6'	2.31	0.43
1:A:233:SER:HB2	1:A:268:ARG:HG2	2.00	0.43
1:B:187:LYS:HB3	1:B:257:LYS:HB3	2.01	0.43
1:B:198:GLY:HA2	1:B:332:SER:OG	2.18	0.43
1:C:195:ASN:OD1	1:C:234:ARG:HG3	2.18	0.43
1:D:72:PHE:CE2	1:D:74:PHE:HB2	2.53	0.43
1:A:7:GLU:HA	1:A:10:GLN:HG3	2.01	0.43
1:A:198:GLY:HA2	1:A:332:SER:OG	2.19	0.42
1:A:33:LEU:HD12	1:A:43:VAL:HG11	2.00	0.42
1:C:177:ALA:HB1	1:C:188:THR:OG1	2.19	0.42
1:D:171:TYR:CE2	1:D:175:ILE:HD11	2.54	0.42
1:A:309:ASP:OD1	1:A:311:THR:HG23	2.18	0.42
1:B:137:PHE:HB3	1:B:188:THR:HG22	2.00	0.42
1:A:119:ILE:HD11	1:A:169:THR:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLN:HG2	1:B:10:GLN:H	1.72	0.42
1:D:79:ILE:HG12	2:D:343:NAD:N1A	2.34	0.42
1:B:156:GLU:HG2	1:B:260:ILE:O	2.19	0.42
1:B:175:ILE:HG22	1:C:168:VAL:HG22	2.01	0.42
1:C:231:GLU:OE2	1:C:231:GLU:HA	2.19	0.42
1:C:5:TYR:CE1	1:C:244:GLN:HA	2.55	0.42
1:D:59:GLU:O	1:D:62:THR:HB	2.19	0.42
1:C:146:TYR:CE1	1:C:154:LYS:HB3	2.55	0.42
1:A:214:TRP:HH2	1:A:271:LEU:HB3	1.85	0.42
1:D:140:ALA:HB1	1:D:193:TYR:CE1	2.54	0.42
1:C:196:VAL:HA	1:C:237:CYS:O	2.20	0.42
1:B:196:VAL:HA	1:B:237:CYS:O	2.20	0.41
1:D:245:MET:HE1	1:D:313:ALA:CB	2.49	0.41
2:C:343:NAD:C5N	3:C:344:UD6:C4'	2.99	0.41
1:C:5:TYR:OH	1:C:35:LYS:HE2	2.20	0.41
1:B:46:LEU:HD22	1:B:88:VAL:HG21	2.02	0.41
1:D:115:ASN:OD1	1:D:119:ILE:HD12	2.21	0.41
1:D:146:TYR:CD1	1:D:159:ILE:HG22	2.56	0.41
1:B:269:THR:HG23	1:B:273:GLU:HG3	2.02	0.41
1:A:14:PHE:CE2	1:B:105:PRO:HB3	2.54	0.41
1:B:196:VAL:HG21	1:B:242:VAL:HG21	2.03	0.41
1:B:165:PRO:O	1:B:169:THR:HG23	2.21	0.41
1:A:1:TYR:N	6:A:352:HOH:O	2.50	0.41
1:C:239:ILE:HG13	1:C:239:ILE:H	1.38	0.41
1:D:239:ILE:H	1:D:239:ILE:HG13	1.49	0.41
1:D:38:LYS:HG3	1:D:64:VAL:HG12	2.03	0.41
1:D:89:MET:O	1:D:90:LYS:C	2.60	0.41
1:B:138:THR:HG21	1:B:249:SER:HB2	2.03	0.40
2:D:343:NAD:C4N	3:D:344:UD6:C4'	2.91	0.40
1:B:171:TYR:CZ	1:B:175:ILE:HD11	2.57	0.40
1:D:83:THR:O	1:D:87:GLN:HG2	2.21	0.40
1:D:22:THR:OG1	1:D:97:HIS:HA	2.21	0.40
1:A:233:SER:HB3	1:A:270:THR:HG22	2.03	0.40
1:B:104:VAL:N	1:B:105:PRO:CD	2.84	0.40
1:C:191:LEU:HB3	1:C:263:VAL:CG2	2.50	0.40
1:B:299:ARG:O	1:B:302:ASP:HB3	2.22	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	332/351 (95%)	312 (94%)	19 (6%)	1 (0%)	41	70
1	B	332/351 (95%)	310 (93%)	21 (6%)	1 (0%)	41	70
1	C	332/351 (95%)	314 (95%)	18 (5%)	0	100	100
1	D	332/351 (95%)	316 (95%)	15 (4%)	1 (0%)	41	70
All	All	1328/1404 (95%)	1252 (94%)	73 (6%)	3 (0%)	47	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	103	SER
1	A	103	SER
1	D	286	HIS

### 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	290/304 (95%)	283 (98%)	7 (2%)	49	78
1	B	290/304 (95%)	281 (97%)	9 (3%)	40	72
1	C	290/304 (95%)	284 (98%)	6 (2%)	53	80
1	D	290/304 (95%)	280 (97%)	10 (3%)	37	69
All	All	1160/1216 (95%)	1128 (97%)	32 (3%)	43	75

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	109	VAL
1	A	213	LYS
1	A	239	ILE
1	A	306	SER
1	A	310	VAL
1	A	338	ARG
1	B	14	PHE
1	B	78	ASP
1	B	117	THR
1	B	199	ARG
1	B	234	ARG
1	B	239	ILE
1	B	293	ILE
1	B	324	LYS
1	B	338	ARG
1	C	65	SER
1	C	176	TYR
1	C	199	ARG
1	C	213	LYS
1	C	239	ILE
1	C	299	ARG
1	D	7	GLU
1	D	15	SER
1	D	51	THR
1	D	65	SER
1	D	109	VAL
1	D	155	VAL
1	D	176	TYR
1	D	199	ARG
1	D	239	ILE
1	D	245	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	272	ASN
1	B	149	HIS
1	B	178	GLN
1	C	149	HIS
1	C	287	HIS
1	D	149	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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$
2	NAD	D	343	-	42,48,48	1.42	4 (9%)	50,73,73	1.34	6 (12%)
2	NAD	C	343	-	42,48,48	1.47	4 (9%)	50,73,73	1.31	7 (14%)
3	UD6	D	344	-	34,41,41	1.78	3 (8%)	41,62,62	1.32	3 (7%)
4	SO4	A	347	-	4,4,4	0.13	0	6,6,6	0.12	0
4	SO4	A	345	-	4,4,4	0.13	0	6,6,6	0.13	0
3	UD6	B	344	-	34,41,41	1.81	4 (11%)	41,62,62	0.96	1 (2%)
3	UD6	C	344	-	34,41,41	1.78	3 (8%)	41,62,62	1.18	2 (4%)
4	SO4	A	346	-	4,4,4	0.16	0	6,6,6	0.09	0
3	UD6	A	344	-	34,41,41	1.88	5 (14%)	41,62,62	1.32	5 (12%)
2	NAD	B	343	-	42,48,48	1.31	5 (11%)	50,73,73	1.22	5 (10%)
2	NAD	A	343	-	42,48,48	1.38	5 (11%)	50,73,73	1.17	4 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	D	343	-	-	5/26/62/62	0/5/5/5
2	NAD	C	343	-	-	9/26/62/62	0/5/5/5
3	UD6	D	344	-	-	12/25/63/63	0/3/3/3
3	UD6	B	344	-	-	11/25/63/63	0/3/3/3
3	UD6	C	344	-	-	10/25/63/63	0/3/3/3
3	UD6	A	344	-	-	7/25/63/63	0/3/3/3
2	NAD	B	343	-	-	3/26/62/62	0/5/5/5
2	NAD	A	343	-	-	12/26/62/62	0/5/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	343	NAD	C2N-N1N	6.85	1.43	1.35
3	B	344	UD6	C9'-C7'	-6.83	1.39	1.51
2	D	343	NAD	C2N-N1N	6.78	1.43	1.35
3	A	344	UD6	C9'-C7'	-6.73	1.39	1.51
3	C	344	UD6	C9'-C7'	-6.72	1.39	1.51
3	D	344	UD6	C9'-C7'	-6.47	1.40	1.51
2	B	343	NAD	C2N-N1N	5.37	1.41	1.35
3	D	344	UD6	C6-N1	4.97	1.42	1.35
3	C	344	UD6	C6-N1	4.90	1.41	1.35
2	A	343	NAD	C2N-N1N	4.53	1.40	1.35
3	A	344	UD6	C6-N1	4.46	1.41	1.35
3	B	344	UD6	C6-N1	4.44	1.41	1.35
3	D	344	UD6	C4-N3	4.25	1.40	1.33
3	A	344	UD6	C4-N3	4.24	1.40	1.33
3	C	344	UD6	C4-N3	4.14	1.40	1.33
3	B	344	UD6	C4-N3	4.13	1.40	1.33
2	A	343	NAD	O4D-C1D	3.68	1.46	1.41
3	A	344	UD6	O4B-C1B	3.54	1.46	1.41
3	B	344	UD6	O4B-C1B	3.13	1.45	1.41
2	A	343	NAD	O4B-C1B	3.00	1.45	1.41
2	A	343	NAD	C3N-C7N	2.77	1.54	1.50
2	C	343	NAD	C6N-N1N	2.73	1.42	1.35
2	C	343	NAD	O4D-C1D	2.69	1.44	1.41
2	B	343	NAD	O4B-C1B	2.55	1.44	1.41
2	D	343	NAD	C6N-N1N	2.44	1.41	1.35
2	B	343	NAD	O4D-C1D	2.38	1.44	1.41
2	A	343	NAD	O5D-C5D	-2.36	1.35	1.44
2	D	343	NAD	C3N-C7N	2.26	1.54	1.50
3	A	344	UD6	O5'-C1'	2.21	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	343	NAD	O4D-C1D	2.18	1.44	1.41
2	B	343	NAD	C3N-C7N	2.17	1.53	1.50
2	B	343	NAD	C6N-N1N	2.16	1.40	1.35
2	C	343	NAD	C3N-C7N	2.07	1.53	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	344	UD6	O5'-C1'-O1'	-4.95	104.90	111.36
2	D	343	NAD	N3A-C2A-N1A	-4.72	121.31	128.68
2	C	343	NAD	N3A-C2A-N1A	-4.58	121.53	128.68
3	C	344	UD6	O3A-PB-O1'	-4.49	93.43	102.48
2	A	343	NAD	N3A-C2A-N1A	-4.41	121.78	128.68
2	B	343	NAD	N3A-C2A-N1A	-4.41	121.78	128.68
3	A	344	UD6	O5'-C5'-C6'	3.97	116.30	106.44
3	A	344	UD6	O5'-C1'-O1'	-3.00	107.45	111.36
3	A	344	UD6	O3A-PB-O1'	-2.97	96.49	102.48
3	D	344	UD6	O3A-PB-O1'	-2.94	96.57	102.48
2	D	343	NAD	PN-O3-PA	-2.85	123.04	132.83
2	C	343	NAD	PN-O3-PA	-2.82	123.14	132.83
3	C	344	UD6	O5'-C1'-O1'	-2.81	107.69	111.36
2	B	343	NAD	O4D-C1D-C2D	-2.81	102.83	106.93
2	D	343	NAD	C3N-C2N-N1N	-2.73	117.76	120.43
2	B	343	NAD	O4B-C1B-C2B	-2.71	102.96	106.93
2	C	343	NAD	C3N-C2N-N1N	-2.68	117.80	120.43
2	A	343	NAD	O4B-C1B-C2B	-2.62	103.09	106.93
2	D	343	NAD	O4B-C1B-C2B	-2.49	103.28	106.93
2	C	343	NAD	O4B-C1B-C2B	-2.49	103.29	106.93
2	D	343	NAD	C3D-C2D-C1D	-2.48	97.25	100.98
3	D	344	UD6	C6'-C5'-C4'	2.41	118.65	113.00
3	A	344	UD6	C2'-C3'-C4'	-2.30	106.80	110.74
2	B	343	NAD	PN-O3-PA	-2.24	125.14	132.83
2	B	343	NAD	C3D-C2D-C1D	-2.24	97.61	100.98
3	B	344	UD6	PB-O3A-PA	-2.22	125.19	132.83
2	C	343	NAD	C3D-C2D-C1D	-2.12	97.78	100.98
2	A	343	NAD	C5D-C4D-C3D	-2.11	107.27	115.18
3	A	344	UD6	PB-O3A-PA	-2.09	125.65	132.83
2	D	343	NAD	C5N-C4N-C3N	2.07	122.79	120.34
2	A	343	NAD	C4A-C5A-N7A	-2.04	107.27	109.40
2	C	343	NAD	O4D-C1D-C2D	-2.03	103.97	106.93
2	C	343	NAD	C3N-C7N-N7N	-2.00	115.34	117.75

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	343	NAD	O4D-C4D-C5D-O5D
2	C	343	NAD	C5B-O5B-PA-O2A
2	C	343	NAD	O4D-C4D-C5D-O5D
3	D	344	UD6	C2B-C1B-N1-C6
3	D	344	UD6	O4B-C1B-N1-C6
3	D	344	UD6	PB-O3A-PA-O5B
3	D	344	UD6	C5B-O5B-PA-O2A
3	D	344	UD6	C1'-O1'-PB-O2B
3	B	344	UD6	C2B-C1B-N1-C6
3	B	344	UD6	O4B-C1B-N1-C6
3	B	344	UD6	C5B-O5B-PA-O1A
3	B	344	UD6	C5B-O5B-PA-O2A
3	C	344	UD6	C2B-C1B-N1-C6
3	C	344	UD6	O4B-C1B-N1-C6
3	C	344	UD6	C5B-O5B-PA-O2A
3	C	344	UD6	C1'-O1'-PB-O2B
3	A	344	UD6	C2B-C1B-N1-C6
3	A	344	UD6	O4B-C1B-N1-C6
2	A	343	NAD	C3D-C4D-C5D-O5D
2	A	343	NAD	O4D-C1D-N1N-C2N
3	D	344	UD6	C4'-C5'-C6'-O6'
3	D	344	UD6	O5'-C5'-C6'-O6'
3	A	344	UD6	O5'-C5'-C6'-O6'
3	A	344	UD6	C3B-C4B-C5B-O5B
2	A	343	NAD	O4D-C4D-C5D-O5D
3	A	344	UD6	C4'-C5'-C6'-O6'
2	D	343	NAD	C3D-C4D-C5D-O5D
2	C	343	NAD	C3D-C4D-C5D-O5D
3	B	344	UD6	C3B-C4B-C5B-O5B
3	B	344	UD6	O4B-C4B-C5B-O5B
3	A	344	UD6	O4B-C4B-C5B-O5B
2	B	343	NAD	O4D-C4D-C5D-O5D
3	D	344	UD6	C1'-O1'-PB-O3A
3	C	344	UD6	C1'-O1'-PB-O3A
2	A	343	NAD	C4N-C3N-C7N-O7N
2	A	343	NAD	C2N-C3N-C7N-O7N
2	A	343	NAD	C4N-C3N-C7N-N7N
2	A	343	NAD	C3B-C4B-C5B-O5B
3	B	344	UD6	O5'-C5'-C6'-O6'
2	B	343	NAD	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	A	343	NAD	O4B-C4B-C5B-O5B
2	A	343	NAD	C2N-C3N-C7N-N7N
2	C	343	NAD	PN-O3-PA-O5B
3	B	344	UD6	PB-O3A-PA-O5B
3	A	344	UD6	PB-O3A-PA-O5B
2	C	343	NAD	C5B-O5B-PA-O3
3	D	344	UD6	C5B-O5B-PA-O3A
3	D	344	UD6	C1'-O1'-PB-O1B
3	C	344	UD6	C1'-O1'-PB-O1B
2	A	343	NAD	PN-O3-PA-O1A
2	C	343	NAD	C5B-O5B-PA-O1A
3	D	344	UD6	C5B-O5B-PA-O1A
3	C	344	UD6	C5B-O5B-PA-O1A
3	B	344	UD6	C1'-O1'-PB-O3A
3	C	344	UD6	O5'-C1'-O1'-PB
2	C	343	NAD	O4B-C4B-C5B-O5B
2	C	343	NAD	PA-O3-PN-O1N
3	C	344	UD6	PB-O3A-PA-O5B
2	D	343	NAD	C5B-O5B-PA-O3
3	B	344	UD6	C5B-O5B-PA-O3A
3	C	344	UD6	C5B-O5B-PA-O3A
3	D	344	UD6	PB-O3A-PA-O2A
3	B	344	UD6	C1'-O1'-PB-O1B
2	A	343	NAD	PN-O3-PA-O2A
2	A	343	NAD	PA-O3-PN-O2N
2	D	343	NAD	C5B-O5B-PA-O1A
2	D	343	NAD	O4B-C4B-C5B-O5B
2	C	343	NAD	C3B-C4B-C5B-O5B
2	B	343	NAD	O4B-C4B-C5B-O5B

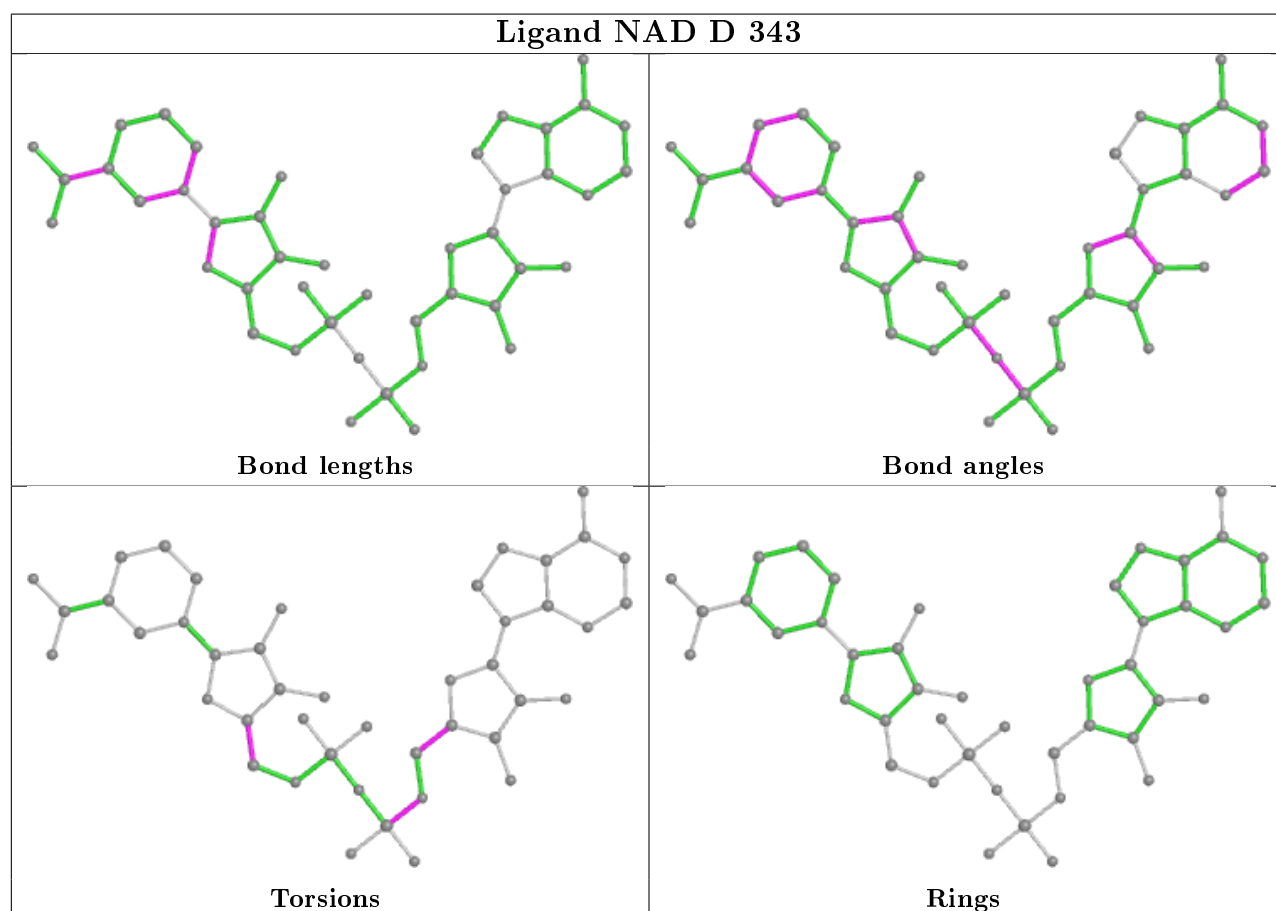
There are no ring outliers.

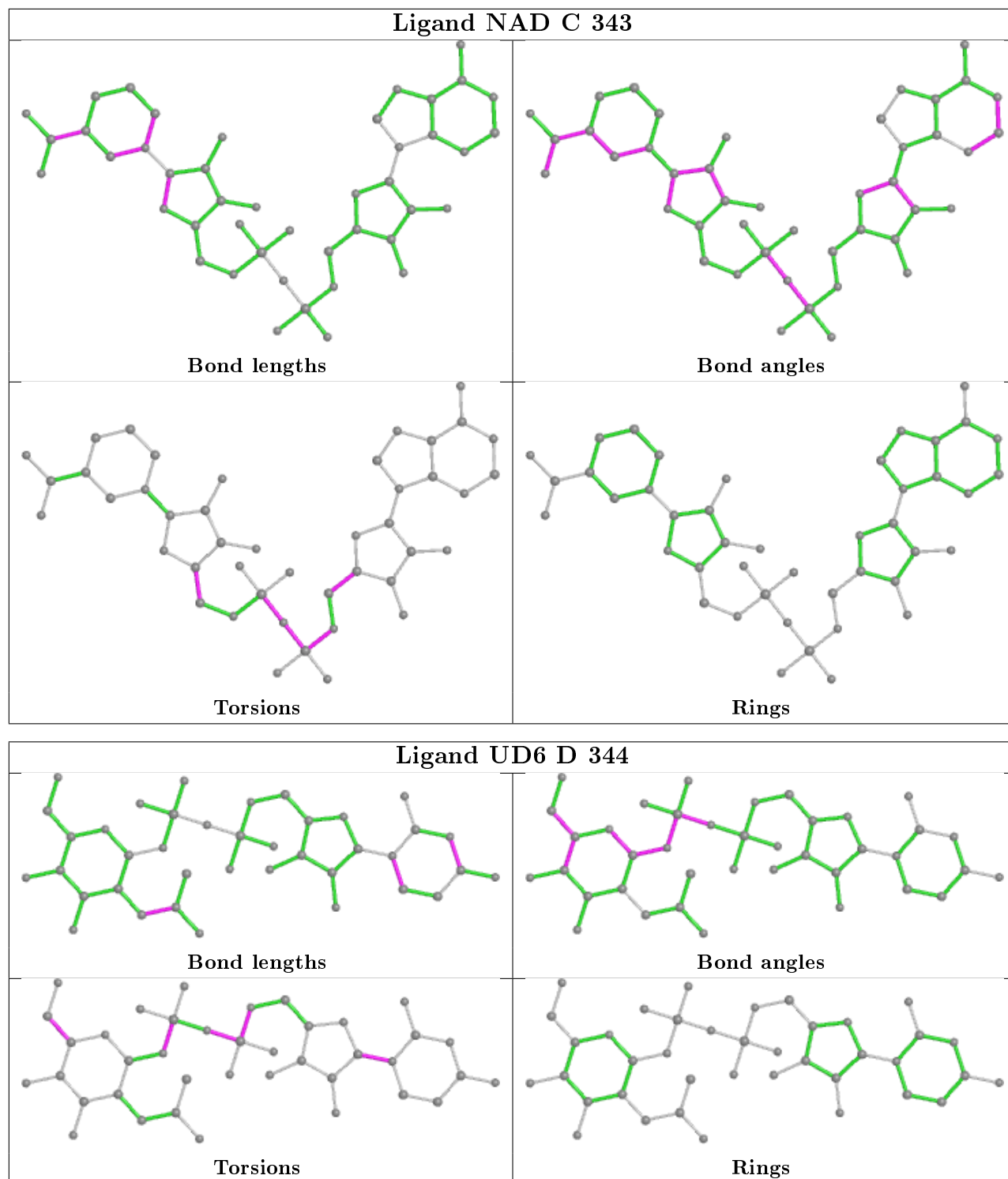
8 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	343	NAD	6	0
2	C	343	NAD	8	0
3	D	344	UD6	5	0
3	B	344	UD6	4	0
3	C	344	UD6	5	0
3	A	344	UD6	4	0
2	B	343	NAD	5	0
2	A	343	NAD	11	0

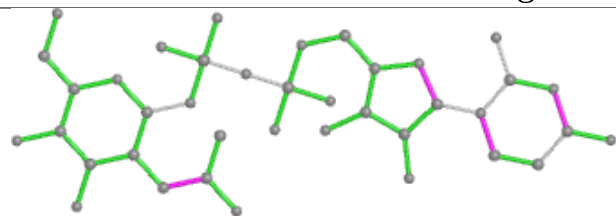


The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

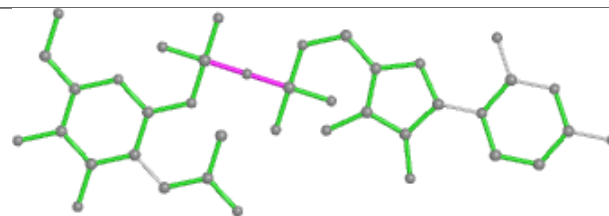




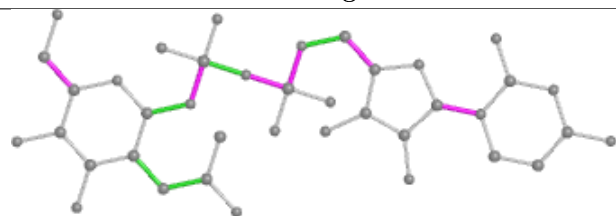
## Ligand UD6 B 344



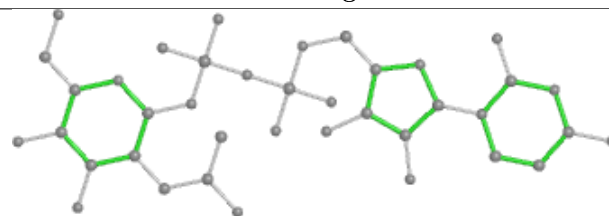
Bond lengths



Bond angles

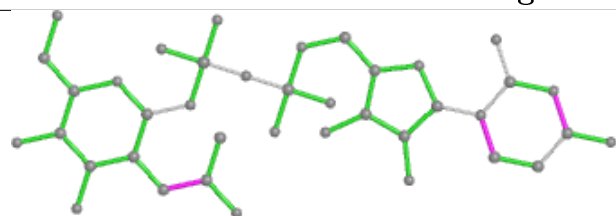


Torsions

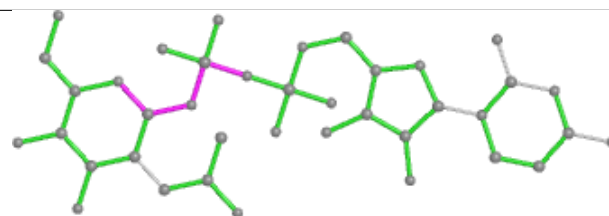


Rings

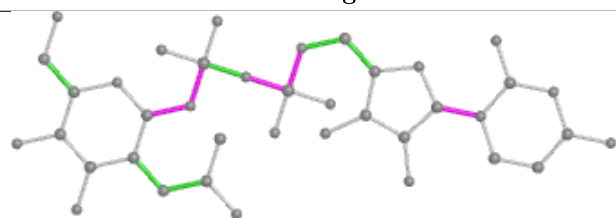
## Ligand UD6 C 344



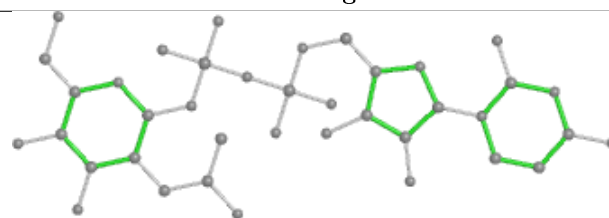
Bond lengths



Bond angles

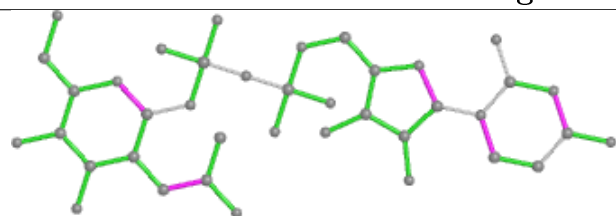


Torsions

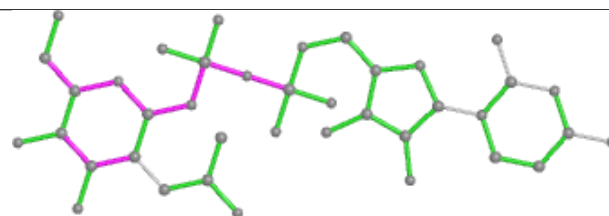


Rings

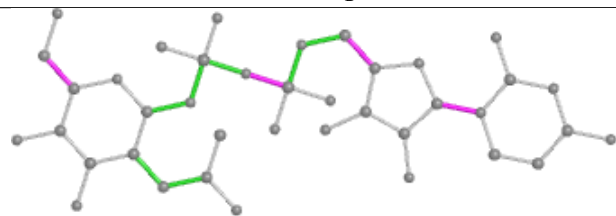
## Ligand UD6 A 344



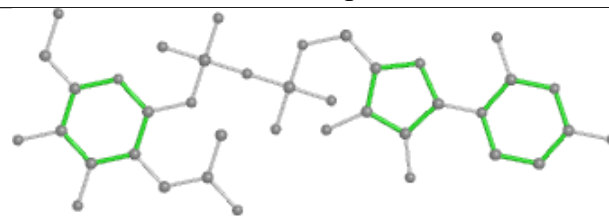
Bond lengths



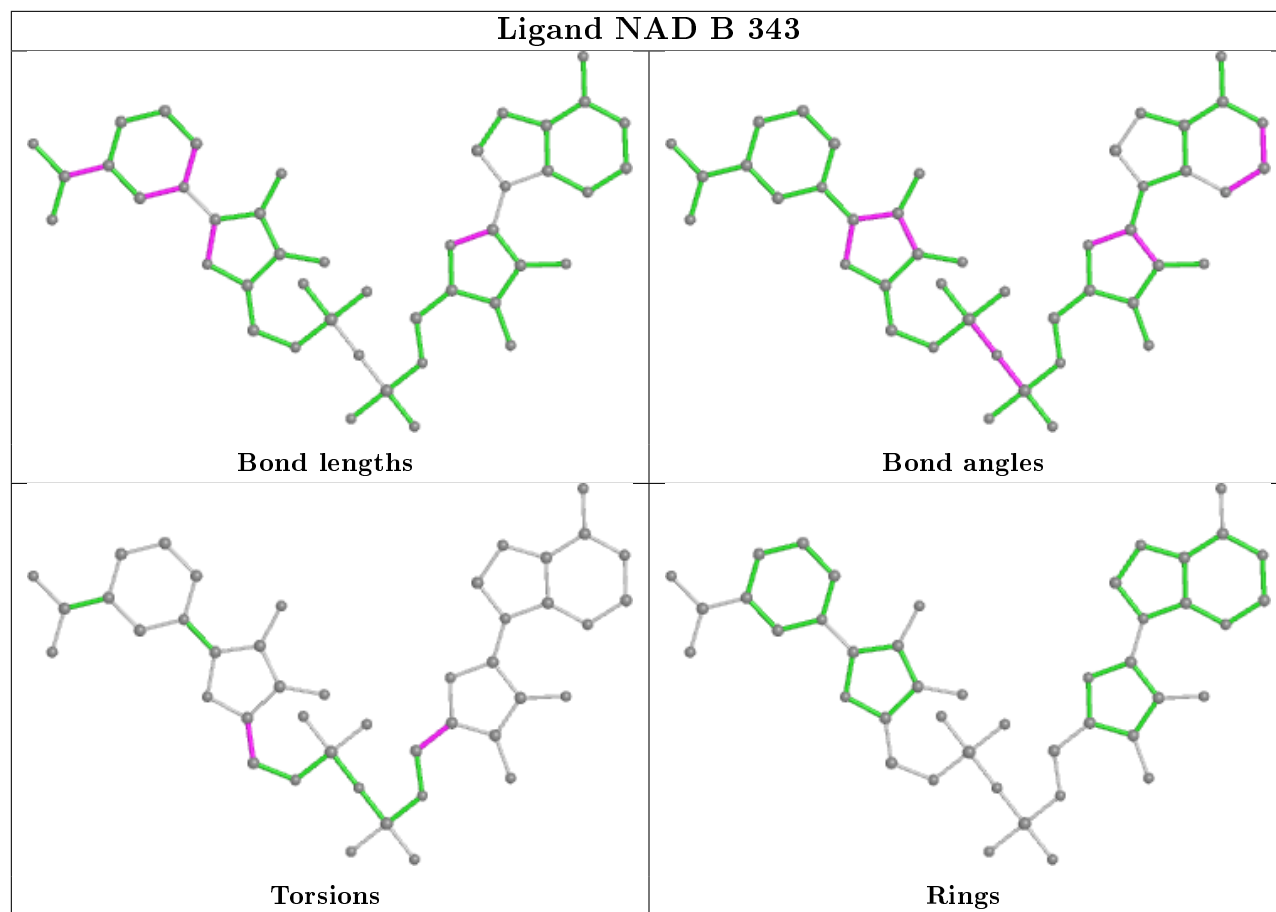
Bond angles

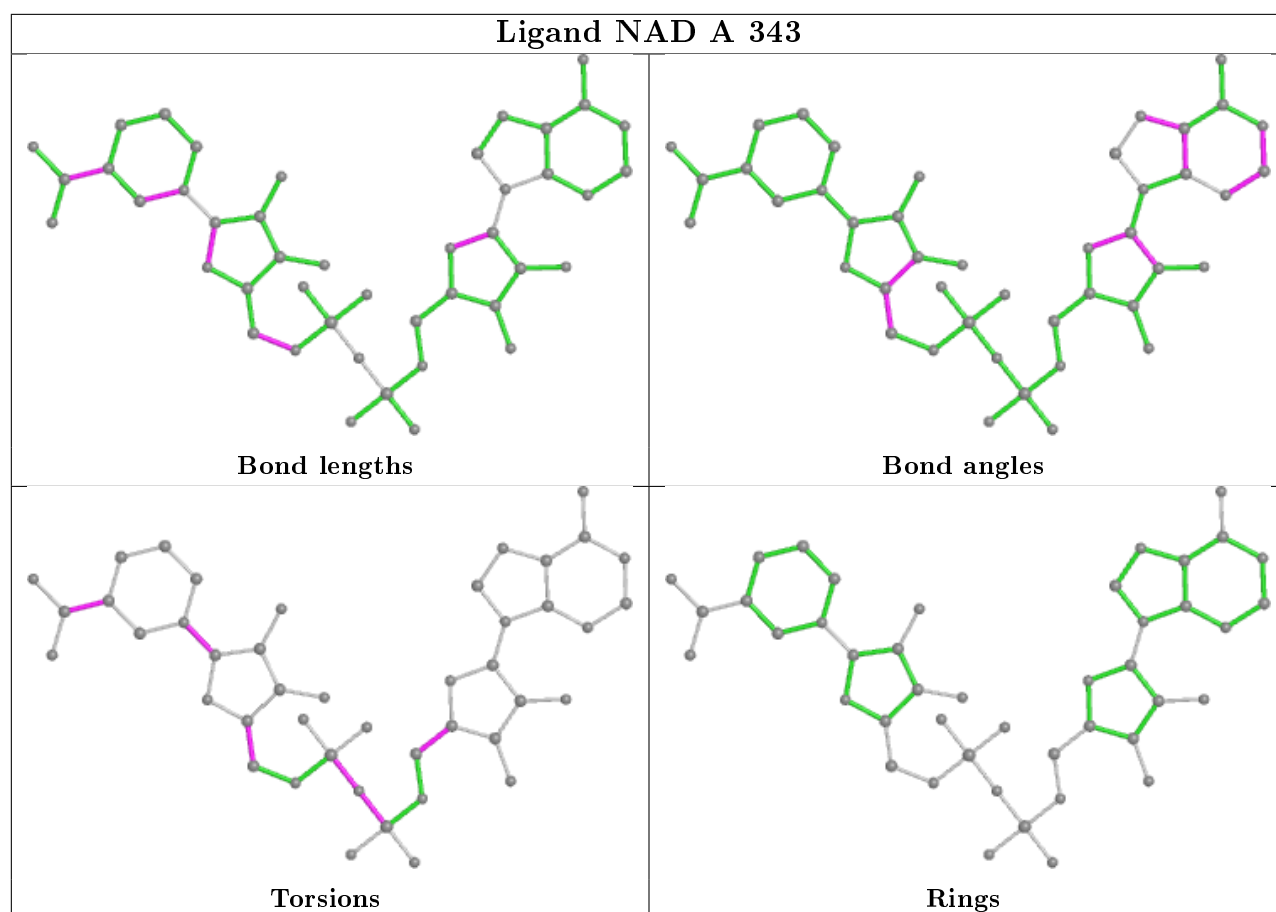


Torsions



Rings





## 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 ⓘ

### 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	336/351 (95%)	-0.01	5 (1%) 73 73	16, 31, 70, 91	0
1	B	336/351 (95%)	0.01	4 (1%) 79 78	16, 31, 69, 93	0
1	C	336/351 (95%)	0.03	5 (1%) 73 73	18, 33, 60, 81	0
1	D	336/351 (95%)	0.05	6 (1%) 68 67	17, 32, 60, 81	0
All	All	1344/1404 (95%)	0.02	20 (1%) 73 73	16, 32, 67, 93	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	286	HIS	7.0
1	D	1	TYR	6.7
1	D	2	MET	5.9
1	C	2	MET	5.6
1	C	1	TYR	4.8
1	A	225	TYR	3.5
1	C	286	HIS	3.5
1	B	286	HIS	3.5
1	A	286	HIS	3.1
1	A	300	SER	3.0
1	B	225	TYR	2.9
1	C	301	GLY	2.7
1	B	284	LEU	2.6
1	D	303	VAL	2.5
1	D	226	ILE	2.5
1	A	298	PHE	2.3
1	A	303	VAL	2.3
1	C	303	VAL	2.0
1	D	301	GLY	2.0
1	B	279	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

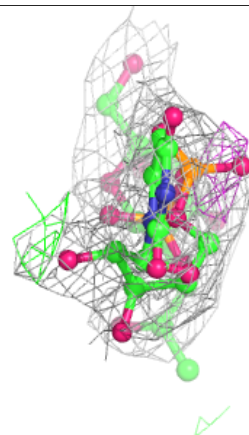
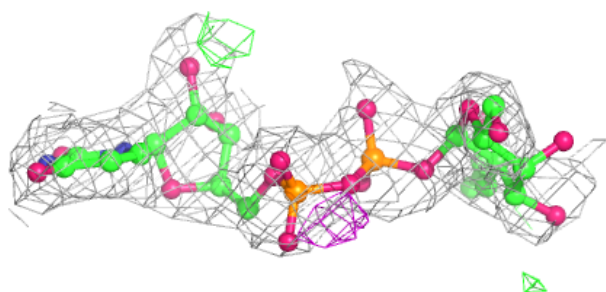
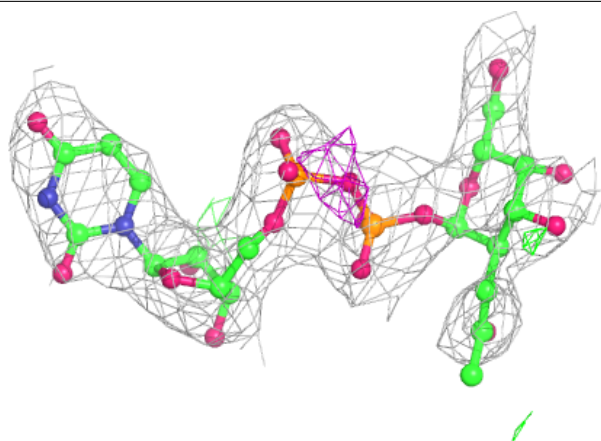
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	347	5/5	0.84	0.22	77,77,77,77	0
3	UD6	B	344	39/39	0.91	0.20	25,37,58,60	14
3	UD6	A	344	39/39	0.94	0.17	27,38,57,59	14
3	UD6	D	344	39/39	0.95	0.19	29,35,44,46	14
3	UD6	C	344	39/39	0.95	0.17	28,33,42,44	14
5	NA	A	348	1/1	0.95	0.21	22,22,22,22	0
2	NAD	D	343	44/44	0.96	0.17	22,28,38,41	0
2	NAD	C	343	44/44	0.96	0.20	21,27,37,38	0
2	NAD	B	343	44/44	0.96	0.18	20,25,37,39	0
2	NAD	A	343	44/44	0.97	0.18	21,24,39,40	0
4	SO4	A	345	5/5	0.98	0.14	38,38,38,39	0
4	SO4	A	346	5/5	0.99	0.15	44,45,45,45	0

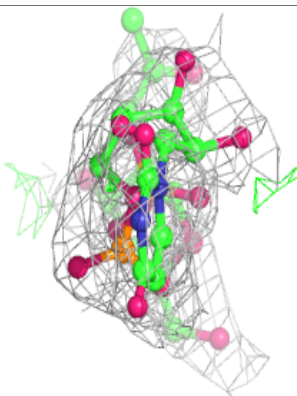
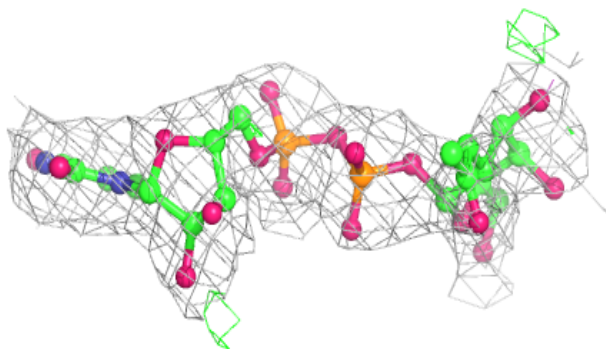
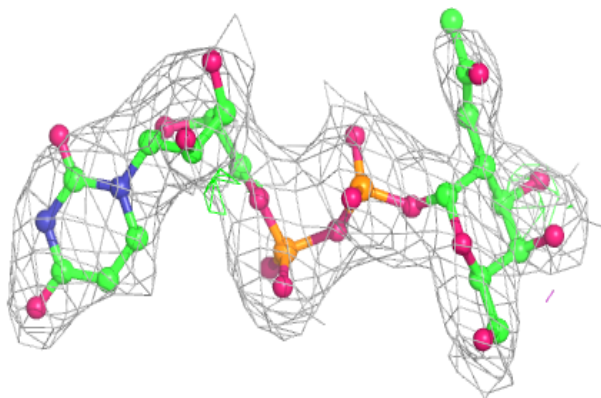
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around UD6 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 UD6 A 344:**

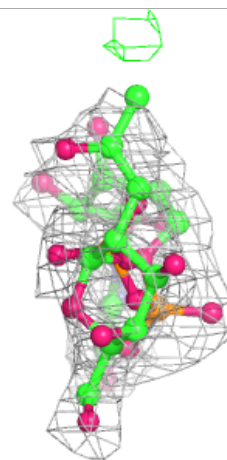
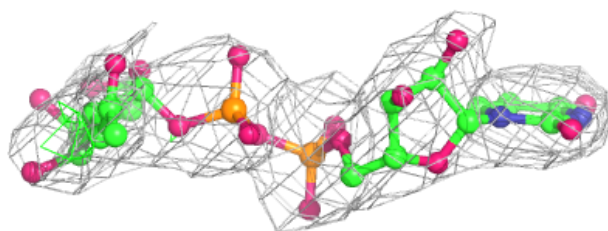
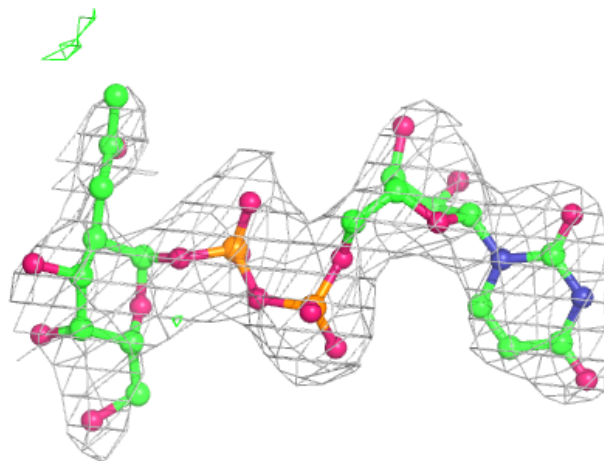
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





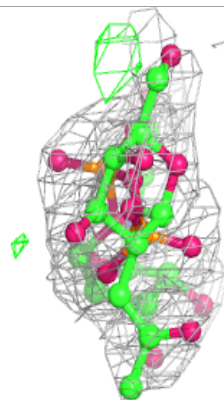
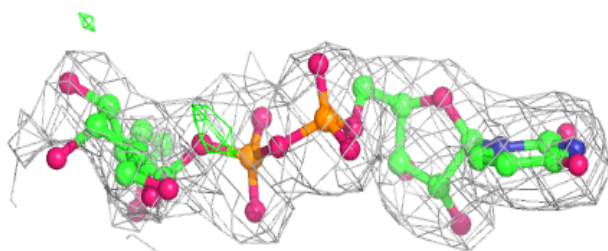
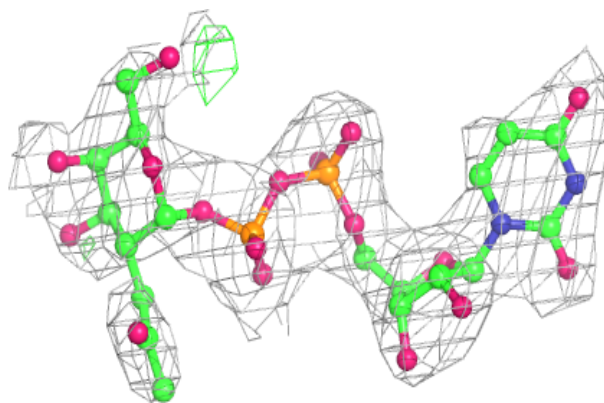
**Electron density around UD6 D 344:**

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

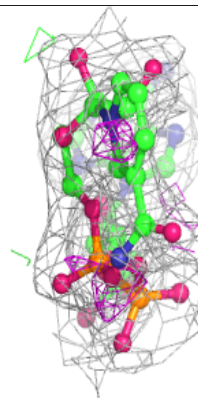
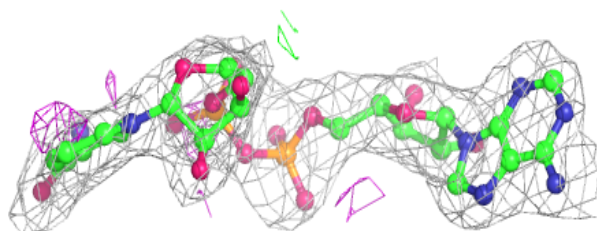
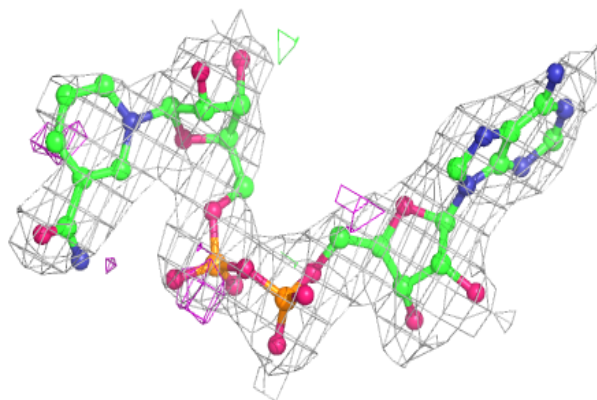


**Electron density around UD6 C 344:**

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

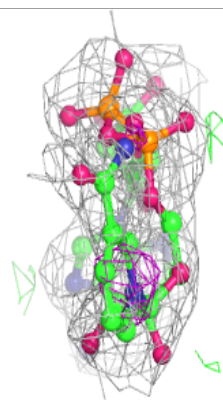
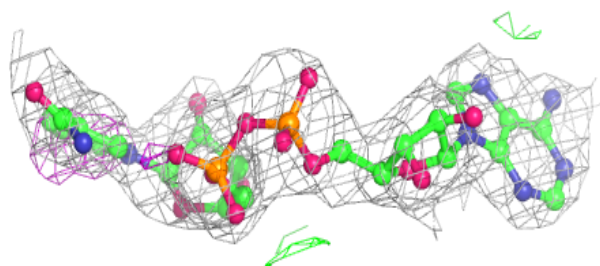
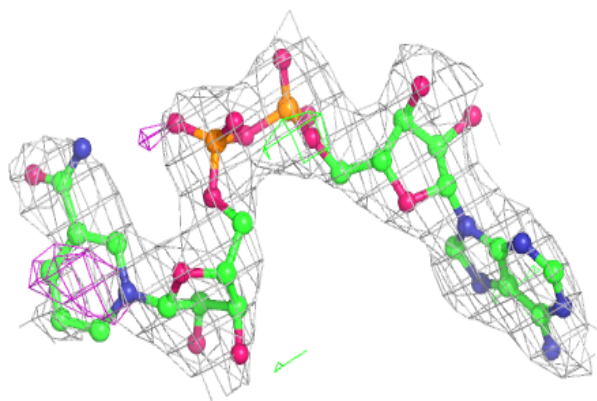
**Electron density around NAD D 343:**

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

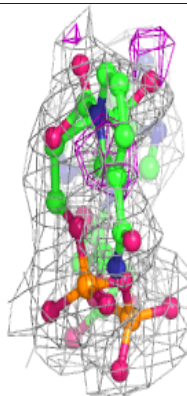
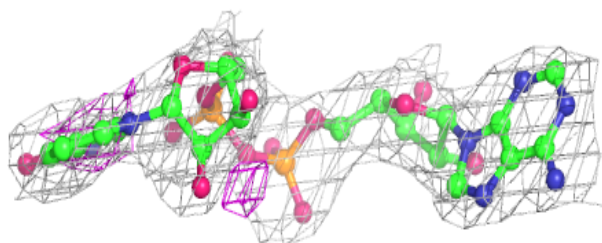
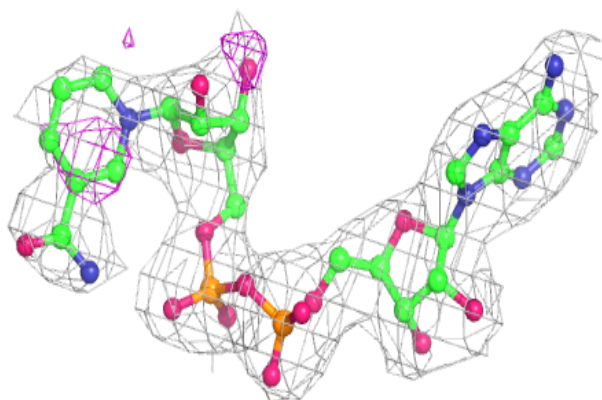


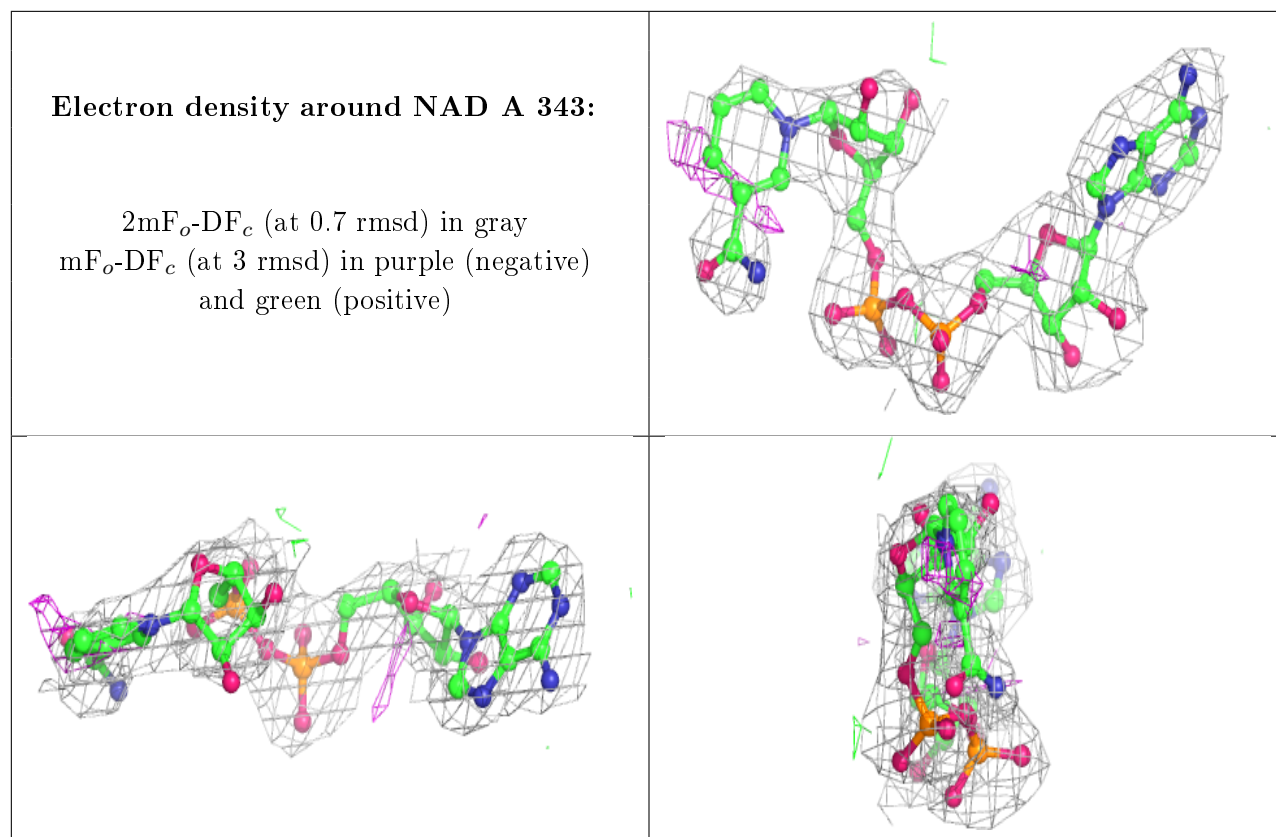
**Electron density around NAD C 343:**

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

**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.