



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 04:16 am BST

PDB ID : 3RUC
Title : Specific recognition of N-acetylated substrates and domain flexibility in WbgU:
a UDP-GalNAc 4-epimerase
Authors : Bhatt, V.S.; Guan, W.; Wang, P.G.
Deposited on : 2011-05-04
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

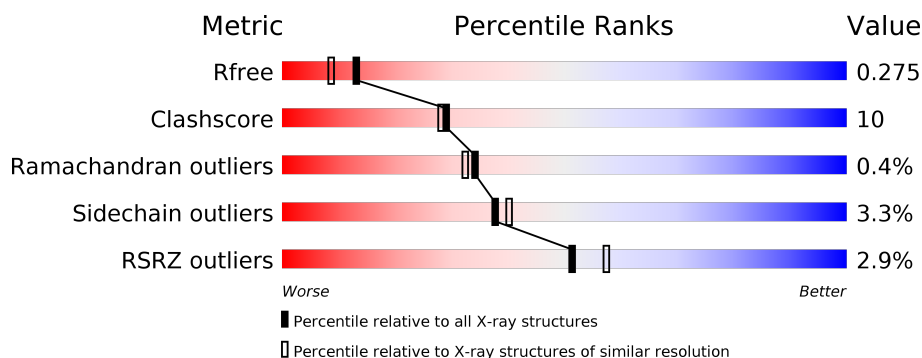
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 ≥ 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>3%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	B	351	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
1	C	351	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• •</div> </div> </div>
1	D	351	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11405 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
			2676	1709	457	502	8			
1	B	336	Total	C	N	O	S	0	0	0
			2676	1709	457	502	8			
1	C	336	Total	C	N	O	S	0	0	0
			2676	1709	457	502	8			
1	D	336	Total	C	N	O	S	0	0	0
			2676	1709	457	502	8			

There are 28 discrepancies between the modelled and reference sequences:

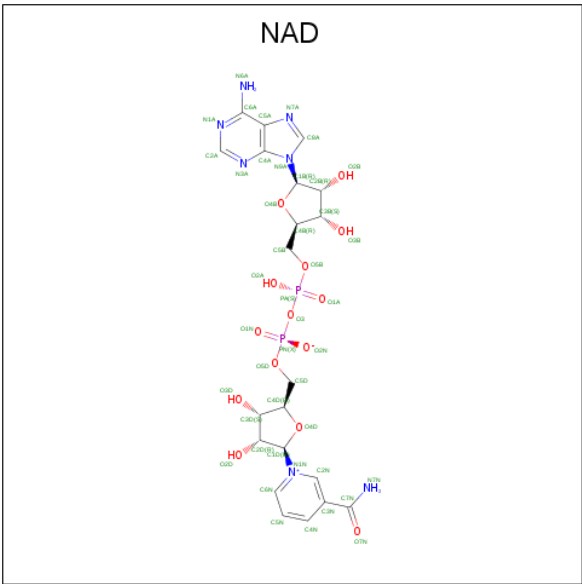
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9
A	305	ALA	HIS	ENGINEERED MUTATION	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
B	305	ALA	HIS	ENGINEERED MUTATION	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
C	305	ALA	HIS	ENGINEERED MUTATION	UNP Q7BJX9

Continued on next page...

Continued from previous page...

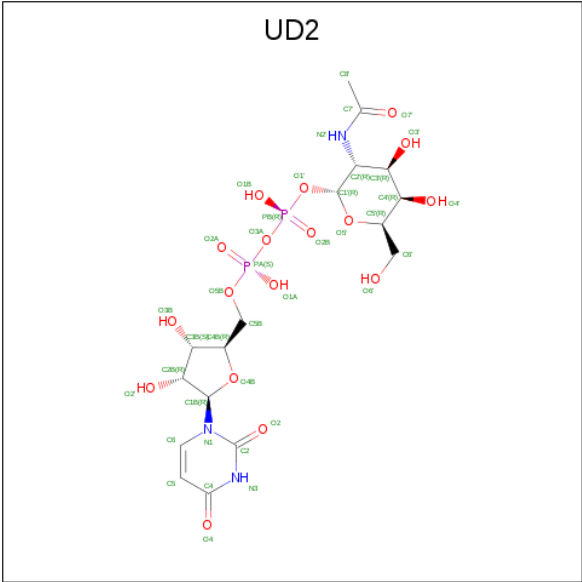
Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-7	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-6	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-5	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-4	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	-3	HIS	-	EXPRESSION TAG	UNP Q7BJX9
D	305	ALA	HIS	ENGINEERED MUTATION	UNP Q7BJX9

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



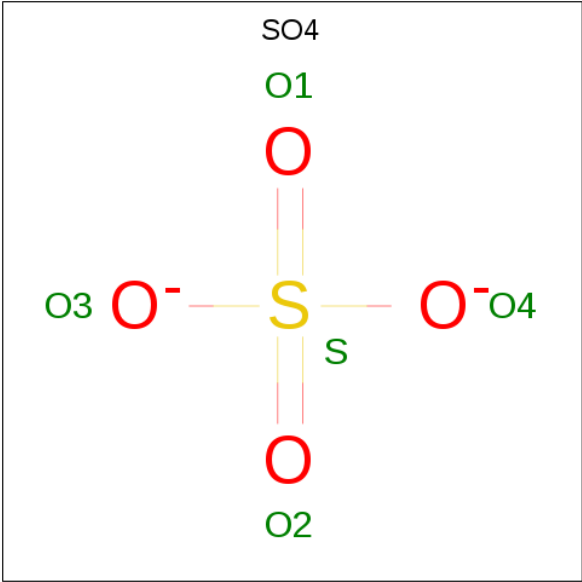
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is URIDINE-DIPHOSPHATE-N-ACETYLGLACTOSAMINE (three-letter code: UD2) (formula: C₁₇H₂₇N₃O₁₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



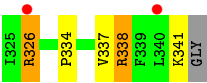
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

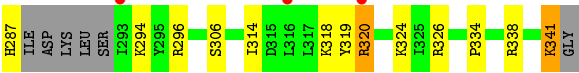
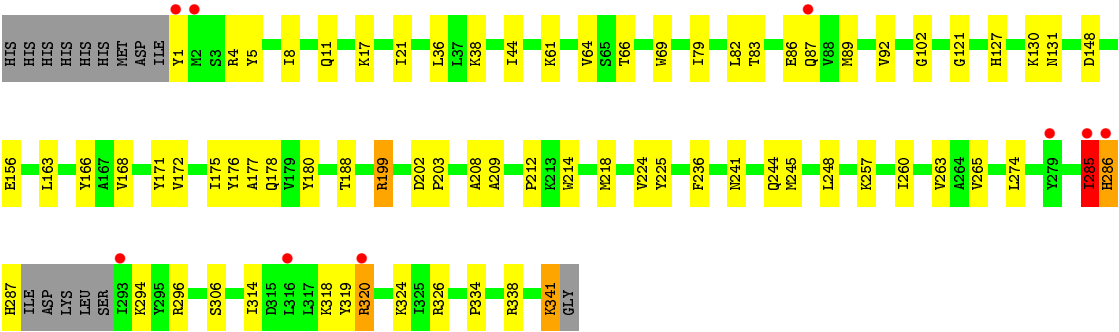
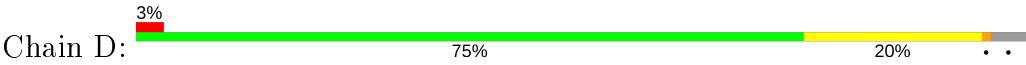
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	92	Total	O	0	0
			92	92		
5	B	80	Total	O	0	0
			80	80		
5	C	91	Total	O	0	0
			91	91		
5	D	96	Total	O	0	0
			96	96		

- Molecule 1: WbgU





● Molecule 1: WbgU



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	78.28 Å 78.28 Å 231.80 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.10 38.59 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.10) 98.8 (38.59-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.215 , 0.270 0.220 , 0.275	Depositor DCC
R_{free} test set	4641 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.105 for -h,-k,l 0.458 for h,-h-k,-l 0.105 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11405	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UD2, 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	0.97	2/2733 (0.1%)	0.86	0/3709
1	B	0.99	2/2733 (0.1%)	0.89	2/3709 (0.1%)
1	C	0.95	0/2733	0.86	6/3709 (0.2%)
1	D	0.95	0/2733	0.87	2/3709 (0.1%)
All	All	0.96	4/10932 (0.0%)	0.87	10/14836 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	HIS	C-O	-6.04	1.11	1.23
1	A	74	PHE	CE2-CZ	5.37	1.47	1.37
1	A	166	TYR	CD2-CE2	5.31	1.47	1.39
1	B	60	VAL	CB-CG2	-5.12	1.42	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	C	200	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	202	ASP	CB-CG-OD1	5.98	123.68	118.30
1	D	202	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	C	200	ARG	NE-CZ-NH2	-5.95	117.33	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	LEU	CA-CB-CG	-5.78	102.00	115.30
1	B	258	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	4	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	315	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	202	ASP	CB-CG-OD2	-5.11	113.70	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	285	ILE	Peptide

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	2676	0	2656	51	0
1	B	2676	0	2656	47	0
1	C	2676	0	2656	50	0
1	D	2676	0	2656	52	0
2	A	44	0	26	6	0
2	B	44	0	26	4	0
2	C	44	0	26	8	0
2	D	44	0	26	5	0
3	A	39	0	25	8	0
3	B	39	0	25	4	0
3	C	39	0	25	6	0
3	D	39	0	25	5	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	92	0	0	1	0
5	B	80	0	0	0	0
5	C	91	0	0	3	0
5	D	96	0	0	3	0
All	All	11405	0	10828	210	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 10.

All (210) 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)
2:C:343:NAD:C4N	3:C:344:UD2:H4'	1.68	1.20
1:C:199:ARG:HH11	1:C:199:ARG:HG3	0.95	1.10
2:D:343:NAD:C4N	3:D:344:UD2:H4'	1.92	0.98
1:C:8:ILE:HG23	1:C:251:LEU:HD22	1.49	0.92
1:C:199:ARG:HG3	1:C:199:ARG:NH1	1.71	0.91
1:C:286:HIS:O	1:C:287:HIS:ND1	2.04	0.91
2:A:343:NAD:C4N	3:A:344:UD2:H4'	2.02	0.90
2:C:343:NAD:H4N	3:C:344:UD2:H4'	1.56	0.85
1:C:286:HIS:O	1:C:287:HIS:CG	2.36	0.79
1:D:178:GLN:NE2	1:D:260:ILE:HD11	2.00	0.77
1:D:285:ILE:HD11	1:D:334:PRO:HG3	1.68	0.76
1:A:234:ARG:NE	3:A:344:UD2:H8'2	2.00	0.75
1:A:285:ILE:HG22	1:A:285:ILE:O	1.87	0.75
2:C:343:NAD:C4N	3:C:344:UD2:C4'	2.59	0.75
2:C:343:NAD:C5N	3:C:344:UD2:H4'	2.17	0.74
1:A:83:THR:O	1:A:87:GLN:HG3	1.86	0.74
1:D:209:ALA:O	1:D:212:PRO:HD2	1.87	0.74
1:D:286:HIS:O	1:D:287:HIS:ND1	2.21	0.73
1:B:178:GLN:NE2	1:B:260:ILE:HD11	2.03	0.72
1:C:285:ILE:O	1:C:286:HIS:HB2	1.87	0.72
1:D:83:THR:HG22	1:D:87:GLN:HE21	1.55	0.72
1:C:8:ILE:HG23	1:C:251:LEU:CD2	2.20	0.72
1:C:178:GLN:NE2	1:C:260:ILE:HD11	2.05	0.72
1:C:326:ARG:HG2	5:C:433:HOH:O	1.89	0.71
1:D:244:GLN:HE22	1:D:320:ARG:H	1.35	0.71
2:D:343:NAD:H4N	3:D:344:UD2:H4'	1.73	0.71
1:C:244:GLN:HE22	1:C:320:ARG:H	1.39	0.70
2:B:343:NAD:C4N	3:B:344:UD2:H4'	2.22	0.69
1:B:244:GLN:HE22	1:B:320:ARG:H	1.40	0.68
1:C:8:ILE:CG2	1:C:251:LEU:HD22	2.21	0.68
1:C:31:ASN:HB3	1:C:243:ILE:HD11	1.75	0.68
1:C:199:ARG:HH11	1:C:199:ARG:CG	1.87	0.68
1:B:44:ILE:HD12	1:B:92:VAL:HG22	1.77	0.66
2:D:343:NAD:C4N	3:D:344:UD2:C4'	2.72	0.66
2:C:343:NAD:C5N	3:C:344:UD2:C4'	2.72	0.66
1:D:286:HIS:O	1:D:287:HIS:CG	2.48	0.66
1:D:338:ARG:HG3	1:D:338:ARG:HH11	1.60	0.65
1:C:338:ARG:HH11	1:C:338:ARG:CG	2.10	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ARG:CB	1:C:338:ARG:HH11	2.10	0.64
1:C:171:TYR:CZ	1:C:175:ILE:HD11	2.34	0.63
1:D:341:LYS:C	1:D:341:LYS:HE2	2.19	0.63
1:A:5:TYR:O	1:A:9:THR:HG23	2.01	0.61
2:A:343:NAD:C4N	3:A:344:UD2:C4'	2.76	0.60
1:A:319:TYR:O	1:A:320:ARG:HD2	2.01	0.60
1:B:193:TYR:HB2	2:B:343:NAD:C5N	2.32	0.60
1:D:127:HIS:HD2	1:D:180:TYR:OH	1.85	0.59
1:C:244:GLN:NE2	1:C:320:ARG:H	1.99	0.59
1:B:102:GLY:O	1:B:103:SER:HB3	2.02	0.59
1:B:83:THR:O	1:B:87:GLN:HG3	2.01	0.59
1:C:40:ASN:ND2	1:C:68:GLN:HE21	2.00	0.59
1:D:83:THR:HG22	1:D:87:GLN:NE2	2.19	0.58
1:D:244:GLN:NE2	1:D:320:ARG:H	2.01	0.57
1:D:178:GLN:HE21	1:D:260:ILE:HD11	1.68	0.57
2:B:343:NAD:C4N	3:B:344:UD2:C4'	2.83	0.57
1:A:61:LYS:HD3	1:A:69:TRP:CE2	2.40	0.57
1:D:199:ARG:H	1:D:199:ARG:HD2	1.69	0.57
1:B:61:LYS:HD3	1:B:69:TRP:CE2	2.40	0.56
1:C:178:GLN:HE21	1:C:260:ILE:HD11	1.67	0.56
1:A:268:ARG:HB2	1:A:307:GLN:HG3	1.86	0.56
1:B:244:GLN:NE2	1:B:320:ARG:H	2.03	0.56
1:A:13:ILE:HG22	1:B:109:VAL:CG2	2.36	0.56
1:B:165:PRO:O	1:B:169:THR:HG23	2.06	0.56
1:C:267:ASP:OD2	1:C:324:LYS:HD3	2.06	0.56
1:C:168:VAL:O	1:C:172:VAL:HG23	2.06	0.56
1:B:178:GLN:HE21	1:B:260:ILE:HD11	1.70	0.55
1:B:75:ILE:HD13	1:B:88:VAL:HG12	1.88	0.55
1:D:44:ILE:HD12	1:D:92:VAL:HG22	1.88	0.55
1:C:199:ARG:CG	1:C:199:ARG:NH1	2.54	0.55
1:B:178:GLN:NE2	1:B:260:ILE:CD1	2.68	0.55
1:C:21:ILE:HD11	1:C:36:LEU:HD12	1.88	0.55
1:B:61:LYS:HD3	1:B:69:TRP:NE1	2.22	0.55
1:B:116:ALA:O	1:B:120:THR:HB	2.06	0.55
1:B:5:TYR:O	1:B:9:THR:HG23	2.07	0.55
1:C:285:ILE:HG21	1:C:337:VAL:HG21	1.87	0.54
1:A:193:TYR:HB2	2:A:343:NAD:C5N	2.38	0.54
1:A:265:VAL:O	1:A:265:VAL:CG1	2.55	0.54
1:A:199:ARG:HG3	1:A:335:TRP:CG	2.42	0.54
1:D:326:ARG:HG3	5:D:416:HOH:O	2.08	0.54
1:A:44:ILE:HD12	1:A:92:VAL:HG22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLN:NE2	1:B:106:ARG:HH11	2.06	0.53
1:A:32:LEU:HD13	1:A:96:LEU:HD13	1.89	0.53
1:C:127:HIS:CD2	1:C:180:TYR:OH	2.62	0.53
1:A:142:SER:HG	3:A:344:UD2:HO4'	1.55	0.53
1:A:199:ARG:HG3	1:A:335:TRP:CD1	2.44	0.53
1:A:114:THR:O	1:A:118:ASN:HB2	2.09	0.53
1:C:148:ASP:HB3	1:C:163:LEU:HD21	1.91	0.53
1:C:100:ALA:HB3	2:C:343:NAD:H3D	1.91	0.53
1:D:168:VAL:O	1:D:172:VAL:HG23	2.08	0.53
1:A:61:LYS:HD3	1:A:69:TRP:CD1	2.44	0.53
1:B:21:ILE:HD11	1:B:36:LEU:HD12	1.91	0.52
1:A:285:ILE:O	1:A:285:ILE:CG2	2.56	0.52
1:D:241:ASN:HB3	1:D:319:TYR:OH	2.09	0.52
1:A:13:ILE:CG2	1:B:109:VAL:CG2	2.87	0.52
1:D:127:HIS:CD2	1:D:180:TYR:OH	2.63	0.52
1:C:127:HIS:HD2	1:C:180:TYR:OH	1.93	0.51
1:C:338:ARG:HB2	1:C:338:ARG:HH11	1.74	0.51
1:C:338:ARG:NH1	1:C:338:ARG:HG3	2.24	0.51
1:A:65:SER:HB2	1:A:67:GLU:OE2	2.11	0.51
1:A:116:ALA:O	1:A:120:THR:HB	2.10	0.50
1:D:21:ILE:HD11	1:D:36:LEU:HD12	1.92	0.50
1:A:61:LYS:HD3	1:A:69:TRP:NE1	2.25	0.50
1:C:66:THR:HG23	5:C:371:HOH:O	2.10	0.50
1:D:130:LYS:CE	1:D:131:ASN:OD1	2.59	0.50
1:B:245:MET:HG3	1:B:263:VAL:HG22	1.94	0.50
1:B:114:THR:O	1:B:118:ASN:HB2	2.12	0.49
2:B:343:NAD:C5N	3:B:344:UD2:O4'	2.60	0.49
1:D:82:LEU:O	1:D:86:GLU:HG3	2.11	0.49
1:B:127:HIS:CD2	1:B:180:TYR:OH	2.66	0.48
1:D:130:LYS:HE2	1:D:131:ASN:OD1	2.13	0.48
1:C:266:GLY:HA2	1:C:308:ALA:O	2.13	0.48
1:D:338:ARG:HG3	1:D:338:ARG:NH1	2.28	0.48
1:A:11:GLN:NE2	1:B:205:GLY:HA2	2.29	0.48
1:B:119:ILE:HD13	1:B:172:VAL:HG11	1.96	0.48
2:A:343:NAD:C3N	3:A:344:UD2:H4'	2.42	0.48
1:D:314:ILE:O	1:D:318:LYS:HA	2.14	0.48
1:C:338:ARG:NH1	1:C:338:ARG:CG	2.71	0.48
1:B:319:TYR:O	1:B:320:ARG:HD2	2.14	0.48
1:B:6:GLU:O	1:B:10:GLN:HG3	2.13	0.47
1:C:82:LEU:O	1:C:86:GLU:HG3	2.14	0.47
1:A:75:ILE:HD13	1:A:88:VAL:HG12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLU:CD	1:B:67:GLU:H	2.17	0.47
2:C:343:NAD:C5N	3:C:344:UD2:O4'	2.63	0.47
1:A:263:VAL:O	1:A:263:VAL:HG12	2.13	0.47
1:D:61:LYS:HD3	1:D:69:TRP:CE2	2.50	0.47
1:B:170:LYS:O	1:B:173:ASN:HB2	2.15	0.47
1:A:21:ILE:HD11	1:A:36:LEU:HD12	1.96	0.47
1:B:114:THR:HG22	1:B:169:THR:HG21	1.97	0.47
1:C:338:ARG:HG3	1:C:338:ARG:HH11	1.81	0.46
1:C:130:LYS:HD2	1:C:184:TYR:CG	2.50	0.46
1:A:44:ILE:HD12	1:A:92:VAL:CG2	2.45	0.46
1:D:148:ASP:HB3	1:D:163:LEU:HD21	1.97	0.46
1:B:130:LYS:HE3	1:B:131:ASN:OD1	2.15	0.46
1:A:178:GLN:NE2	1:A:260:ILE:CD1	2.78	0.46
1:A:103:SER:OG	1:A:105:PRO:HD2	2.16	0.46
1:D:245:MET:HG3	1:D:263:VAL:HG22	1.98	0.46
1:A:203:PRO:HA	1:A:212:PRO:HB2	1.98	0.46
1:D:225:TYR:CD1	1:D:296:ARG:HD3	2.50	0.45
1:A:148:ASP:OD1	1:A:161:ASN:N	2.41	0.45
1:D:257:LYS:HE2	5:D:417:HOH:O	2.16	0.45
2:D:343:NAD:C5N	3:D:344:UD2:C4'	2.95	0.45
2:D:343:NAD:C5N	3:D:344:UD2:O4'	2.65	0.45
1:A:37:LEU:O	1:A:68:GLN:HG2	2.17	0.45
1:C:46:LEU:HD22	1:C:88:VAL:HG21	1.99	0.45
1:D:224:VAL:O	1:D:294:LYS:N	2.36	0.45
1:B:188:THR:O	1:B:258:ASP:N	2.50	0.45
1:A:11:GLN:HE22	1:B:205:GLY:HA2	1.82	0.45
1:A:142:SER:HA	2:A:343:NAD:H5N	1.98	0.45
1:A:265:VAL:O	1:A:265:VAL:HG13	2.17	0.45
1:B:199:ARG:HE	1:B:335:TRP:HB2	1.82	0.44
1:D:38:LYS:HG3	1:D:64:VAL:HG12	1.99	0.44
1:B:104:VAL:HB	1:B:105:PRO:HD3	1.98	0.44
1:D:208:ALA:HA	5:D:420:HOH:O	2.16	0.44
1:B:285:ILE:HG21	1:B:337:VAL:HG21	2.00	0.44
1:C:285:ILE:HD11	1:C:334:PRO:HG3	1.99	0.44
1:B:127:HIS:HD2	1:B:180:TYR:OH	2.00	0.44
1:B:178:GLN:HE21	1:B:260:ILE:CD1	2.30	0.44
1:D:177:ALA:HB1	1:D:188:THR:OG1	2.18	0.44
1:A:196:VAL:HA	1:A:237:CYS:O	2.18	0.44
1:D:236:PHE:CZ	1:D:274:LEU:HD22	2.53	0.44
1:D:199:ARG:H	1:D:199:ARG:CD	2.17	0.44
1:D:265:VAL:HG11	1:D:324:LYS:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLN:HE21	1:B:248:LEU:HD11	1.82	0.44
1:D:8:ILE:HA	1:D:8:ILE:HD13	1.85	0.44
1:D:8:ILE:O	1:D:11:GLN:HB2	2.19	0.43
1:A:13:ILE:HG22	1:B:109:VAL:HG21	1.99	0.43
1:D:214:TRP:O	1:D:218:MET:HG3	2.18	0.43
1:D:225:TYR:HA	1:D:294:LYS:O	2.19	0.43
1:B:202:ASP:OD2	1:B:204:ASN:O	2.37	0.43
1:B:234:ARG:NE	3:B:344:UD2:H8'2	2.34	0.43
1:A:244:GLN:HE21	1:A:248:LEU:HD11	1.83	0.43
1:A:10:GLN:NE2	1:B:106:ARG:HD3	2.34	0.43
1:C:140:ALA:O	1:C:170:LYS:NZ	2.47	0.43
1:C:178:GLN:NE2	1:C:260:ILE:CD1	2.80	0.43
1:D:203:PRO:HA	1:D:212:PRO:HB2	1.99	0.43
1:A:165:PRO:O	1:A:169:THR:HG23	2.19	0.43
1:C:20:LEU:HB2	1:C:92:VAL:HG21	2.01	0.42
1:A:244:GLN:NE2	1:A:320:ARG:H	2.17	0.42
1:B:199:ARG:HB3	1:B:335:TRP:CD1	2.54	0.42
1:C:100:ALA:HB3	2:C:343:NAD:C3D	2.49	0.42
1:A:178:GLN:NE2	1:A:260:ILE:HD11	2.34	0.42
1:C:199:ARG:H	1:C:199:ARG:HG2	1.60	0.42
1:D:244:GLN:HE21	1:D:248:LEU:HD11	1.85	0.42
1:D:5:TYR:CE1	1:D:244:GLN:HA	2.55	0.42
1:C:40:ASN:HD21	1:C:68:GLN:HE21	1.65	0.42
1:D:79:ILE:HG13	1:D:121:GLY:HA3	2.00	0.42
1:D:171:TYR:CZ	1:D:175:ILE:HD11	2.55	0.42
1:A:7:GLU:OE1	5:A:396:HOH:O	2.22	0.42
1:A:199:ARG:O	1:A:200:ARG:HB2	2.20	0.42
1:C:264:ALA:HB3	1:C:308:ALA:HB3	2.02	0.42
1:D:178:GLN:HE22	1:D:260:ILE:HD11	1.78	0.42
1:D:285:ILE:O	1:D:286:HIS:HB2	2.20	0.42
1:B:286:HIS:O	1:B:287:HIS:CG	2.73	0.41
2:A:343:NAD:H4N	3:A:344:UD2:H4'	1.95	0.41
1:A:11:GLN:NE2	1:B:206:ALA:H	2.18	0.41
1:D:286:HIS:O	1:D:287:HIS:CE1	2.73	0.41
1:A:286:HIS:O	1:A:287:HIS:CG	2.73	0.41
1:C:314:ILE:O	1:C:318:LYS:HA	2.20	0.41
1:D:156:GLU:HG2	1:D:260:ILE:O	2.19	0.41
1:A:234:ARG:CZ	3:A:344:UD2:H8'2	2.48	0.41
1:A:166:TYR:CZ	3:A:344:UD2:H6'1	2.55	0.41
1:C:285:ILE:CG2	1:C:337:VAL:HG21	2.51	0.41
1:B:319:TYR:C	1:B:320:ARG:HD2	2.42	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:GLY:HA2	1:D:166:TYR:CE1	2.56	0.41
1:A:229:ASP:OD1	1:A:229:ASP:N	2.51	0.41
1:C:167:ALA:HA	5:C:404:HOH:O	2.21	0.40
1:A:285:ILE:HG21	1:A:337:VAL:HG21	2.02	0.40
1:B:283:ASN:O	1:B:286:HIS:CE1	2.74	0.40
1:C:130:LYS:HE2	1:C:130:LYS:HB3	1.89	0.40
1:C:203:PRO:HA	1:C:212:PRO:HB2	2.03	0.40
1:D:61:LYS:HD3	1:D:69:TRP:NE1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/351 (95%)	320 (96%)	11 (3%)	1 (0%)	41	41
1	B	332/351 (95%)	321 (97%)	10 (3%)	1 (0%)	41	41
1	C	332/351 (95%)	320 (96%)	10 (3%)	2 (1%)	25	21
1	D	332/351 (95%)	320 (96%)	11 (3%)	1 (0%)	41	41
All	All	1328/1404 (95%)	1281 (96%)	42 (3%)	5 (0%)	34	32

All (5) Ramachandran outliers are listed below:

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

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	289/303 (95%)	283 (98%)	6 (2%)	53	59
1	B	289/303 (95%)	279 (96%)	10 (4%)	36	38
1	C	289/303 (95%)	277 (96%)	12 (4%)	30	30
1	D	289/303 (95%)	279 (96%)	10 (4%)	36	38
All	All	1156/1212 (95%)	1118 (97%)	38 (3%)	38	40

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	GLU
1	A	176	TYR
1	A	304	ARG
1	A	325	ILE
1	A	338	ARG
1	A	341	LYS
1	B	199	ARG
1	B	265	VAL
1	B	285	ILE
1	B	294	LYS
1	B	297	GLU
1	B	300	SER
1	B	318	LYS
1	B	320	ARG
1	B	338	ARG
1	B	341	LYS
1	C	1	TYR
1	C	4	ARG
1	C	66	THR
1	C	89	MET
1	C	176	TYR
1	C	179	VAL
1	C	199	ARG
1	C	283	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	320	ARG
1	C	326	ARG
1	C	338	ARG
1	C	341	LYS
1	D	1	TYR
1	D	17	LYS
1	D	66	THR
1	D	89	MET
1	D	176	TYR
1	D	199	ARG
1	D	285	ILE
1	D	306	SER
1	D	320	ARG
1	D	341	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	11	GLN
1	A	53	HIS
1	A	127	HIS
1	A	173	ASN
1	A	178	GLN
1	A	244	GLN
1	A	283	ASN
1	B	10	GLN
1	B	11	GLN
1	B	127	HIS
1	B	149	HIS
1	B	173	ASN
1	B	178	GLN
1	B	244	GLN
1	C	40	ASN
1	C	127	HIS
1	C	149	HIS
1	C	178	GLN
1	C	244	GLN
1	D	87	GLN
1	D	127	HIS
1	D	149	HIS
1	D	178	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	244	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	UD2	D	344	-	34,41,41	0.59	0	45,62,62	1.34	5 (11%)
3	UD2	B	344	-	34,41,41	0.79	0	45,62,62	1.38	7 (15%)
4	SO4	A	345	-	4,4,4	0.32	0	6,6,6	0.60	0
2	NAD	C	343	-	42,48,48	1.19	3 (7%)	50,73,73	1.74	8 (16%)
2	NAD	D	343	-	42,48,48	1.25	4 (9%)	50,73,73	1.69	9 (18%)
2	NAD	A	343	-	42,48,48	1.02	3 (7%)	50,73,73	1.62	9 (18%)
2	NAD	B	343	-	42,48,48	0.87	1 (2%)	50,73,73	1.64	11 (22%)
4	SO4	B	345	-	4,4,4	0.13	0	6,6,6	0.85	0
3	UD2	C	344	-	34,41,41	0.59	0	45,62,62	1.41	4 (8%)
3	UD2	A	344	-	34,41,41	0.76	0	45,62,62	1.35	6 (13%)

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	D	344	-	-	5/24/63/63	0/3/3/3
3	UD2	B	344	-	-	5/24/63/63	0/3/3/3
2	NAD	C	343	-	-	4/26/62/62	0/5/5/5
2	NAD	D	343	-	-	4/26/62/62	0/5/5/5
2	NAD	A	343	-	-	5/26/62/62	0/5/5/5
2	NAD	B	343	-	-	6/26/62/62	0/5/5/5
3	UD2	C	344	-	-	5/24/63/63	0/3/3/3
3	UD2	A	344	-	-	7/24/63/63	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	343	NAD	O4B-C1B	4.84	1.47	1.41
2	C	343	NAD	O4B-C1B	3.50	1.46	1.41
2	C	343	NAD	C2A-N3A	3.36	1.37	1.32
2	D	343	NAD	C2B-C1B	-3.03	1.49	1.53
2	C	343	NAD	C2B-C1B	-2.97	1.49	1.53
2	D	343	NAD	C2A-N3A	2.83	1.36	1.32
2	B	343	NAD	O4B-C1B	2.58	1.44	1.41
2	D	343	NAD	O7N-C7N	-2.53	1.19	1.24
2	A	343	NAD	O4D-C1D	2.53	1.44	1.41
2	A	343	NAD	O4B-C1B	2.53	1.44	1.41
2	A	343	NAD	C4A-N3A	2.41	1.39	1.35

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	343	NAD	O7N-C7N-C3N	-5.81	112.67	119.63
2	A	343	NAD	N3A-C2A-N1A	-5.42	120.20	128.68
2	D	343	NAD	N3A-C2A-N1A	-5.34	120.33	128.68
2	B	343	NAD	N3A-C2A-N1A	-5.19	120.57	128.68
3	C	344	UD2	O3A-PB-O1'	-5.06	92.29	102.48
2	D	343	NAD	O7N-C7N-C3N	-4.71	114.00	119.63
2	C	343	NAD	N3A-C2A-N1A	-4.69	121.34	128.68
3	C	344	UD2	C3'-C2'-N2'	-4.52	102.09	110.62
3	B	344	UD2	O3A-PB-O1'	-4.36	93.70	102.48
2	A	343	NAD	C3D-C2D-C1D	-4.11	94.78	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	344	UD2	O5'-C1'-O1'	-3.87	106.31	111.36
2	D	343	NAD	C3N-C7N-N7N	3.86	122.39	117.75
3	D	344	UD2	O3A-PB-O1'	-3.67	95.08	102.48
2	C	343	NAD	C3N-C7N-N7N	3.53	121.99	117.75
3	A	344	UD2	O5'-C1'-O1'	3.49	115.92	111.36
3	B	344	UD2	C3'-C4'-C5'	3.17	115.90	110.24
2	C	343	NAD	C3N-C2N-N1N	-3.15	117.35	120.43
3	D	344	UD2	C3'-C2'-N2'	-3.12	104.73	110.62
2	B	343	NAD	O2N-PN-O1N	3.07	127.41	112.24
3	A	344	UD2	O3A-PB-O1'	-3.06	96.32	102.48
3	A	344	UD2	O4'-C4'-C3'	-3.00	103.42	110.35
2	C	343	NAD	C6N-N1N-C2N	2.99	124.71	121.97
2	B	343	NAD	C3N-C7N-N7N	2.94	121.27	117.75
2	D	343	NAD	O3D-C3D-C4D	-2.89	102.70	111.05
2	B	343	NAD	O4D-C1D-C2D	-2.88	102.71	106.93
2	A	343	NAD	O2N-PN-O1N	2.88	126.50	112.24
2	B	343	NAD	O2B-C2B-C1B	2.86	121.40	110.85
3	B	344	UD2	O5'-C1'-O1'	2.83	115.06	111.36
2	A	343	NAD	C3N-C7N-N7N	2.82	121.13	117.75
2	B	343	NAD	O3D-C3D-C4D	-2.76	103.08	111.05
2	D	343	NAD	O4D-C1D-C2D	-2.61	103.11	106.93
2	D	343	NAD	C2A-N1A-C6A	2.56	123.13	118.75
2	C	343	NAD	O5B-C5B-C4B	-2.54	100.26	108.99
2	C	343	NAD	N6A-C6A-N1A	2.53	123.83	118.57
2	C	343	NAD	O3D-C3D-C4D	-2.50	103.83	111.05
3	A	344	UD2	C3'-C4'-C5'	2.49	114.69	110.24
2	A	343	NAD	O3D-C3D-C4D	-2.49	103.86	111.05
3	B	344	UD2	PB-O3A-PA	-2.48	124.32	132.83
2	B	343	NAD	C1B-N9A-C4A	-2.43	122.37	126.64
2	B	343	NAD	C4A-C5A-N7A	-2.42	106.87	109.40
2	A	343	NAD	C4A-C5A-N7A	-2.41	106.89	109.40
2	D	343	NAD	N6A-C6A-N1A	2.31	123.37	118.57
2	A	343	NAD	O7N-C7N-N7N	-2.31	119.30	122.58
2	D	343	NAD	O2N-PN-O1N	2.30	123.60	112.24
3	C	344	UD2	C2'-N2'-C7'	-2.28	117.64	123.18
3	C	344	UD2	O5'-C1'-C2'	-2.25	106.18	110.58
2	B	343	NAD	O5B-PA-O1A	-2.24	100.30	109.07
3	B	344	UD2	O3B-C3B-C2B	-2.23	104.61	111.82
3	D	344	UD2	C3'-C4'-C5'	2.23	114.21	110.24
3	D	344	UD2	C2'-N2'-C7'	-2.17	117.90	123.18
3	A	344	UD2	O3'-C3'-C4'	-2.16	105.34	110.35
2	B	343	NAD	C2A-N1A-C6A	2.16	122.46	118.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	343	NAD	O2D-C2D-C1D	2.14	118.75	110.85
2	A	343	NAD	C2A-N1A-C6A	2.13	122.40	118.75
3	B	344	UD2	O4'-C4'-C3'	-2.13	105.43	110.35
2	A	343	NAD	O4D-C4D-C5D	2.12	116.35	109.37
3	B	344	UD2	O5'-C1'-C2'	-2.10	106.48	110.58
2	D	343	NAD	C5B-C4B-C3B	-2.04	107.53	115.18
3	A	344	UD2	PB-O3A-PA	-2.01	125.91	132.83

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	344	UD2	C2B-C1B-N1-C6
3	D	344	UD2	O4B-C1B-N1-C6
3	B	344	UD2	C2B-C1B-N1-C6
3	B	344	UD2	O4B-C1B-N1-C6
2	C	343	NAD	C5D-O5D-PN-O1N
2	D	343	NAD	C5D-O5D-PN-O1N
2	A	343	NAD	C5D-O5D-PN-O1N
2	B	343	NAD	PN-O3-PA-O5B
2	B	343	NAD	C5D-O5D-PN-O1N
2	B	343	NAD	C5D-O5D-PN-O2N
3	C	344	UD2	C2B-C1B-N1-C6
3	C	344	UD2	O4B-C1B-N1-C6
3	A	344	UD2	C2B-C1B-N1-C6
3	A	344	UD2	O4B-C1B-N1-C6
3	B	344	UD2	O4B-C4B-C5B-O5B
3	A	344	UD2	O4B-C4B-C5B-O5B
3	B	344	UD2	C3B-C4B-C5B-O5B
3	C	344	UD2	PB-O3A-PA-O2A
3	D	344	UD2	PB-O3A-PA-O5B
3	B	344	UD2	PB-O3A-PA-O5B
2	A	343	NAD	PN-O3-PA-O5B
3	C	344	UD2	PB-O3A-PA-O5B
3	A	344	UD2	PB-O3A-PA-O5B
3	D	344	UD2	C4'-C5'-C6'-O6'
2	C	343	NAD	C5D-O5D-PN-O3
2	A	343	NAD	C5D-O5D-PN-O3
3	A	344	UD2	C3B-C4B-C5B-O5B
2	B	343	NAD	PA-O3-PN-O1N
2	C	343	NAD	C5D-O5D-PN-O2N
2	D	343	NAD	C5D-O5D-PN-O2N

Continued on next page...

Continued from previous page...

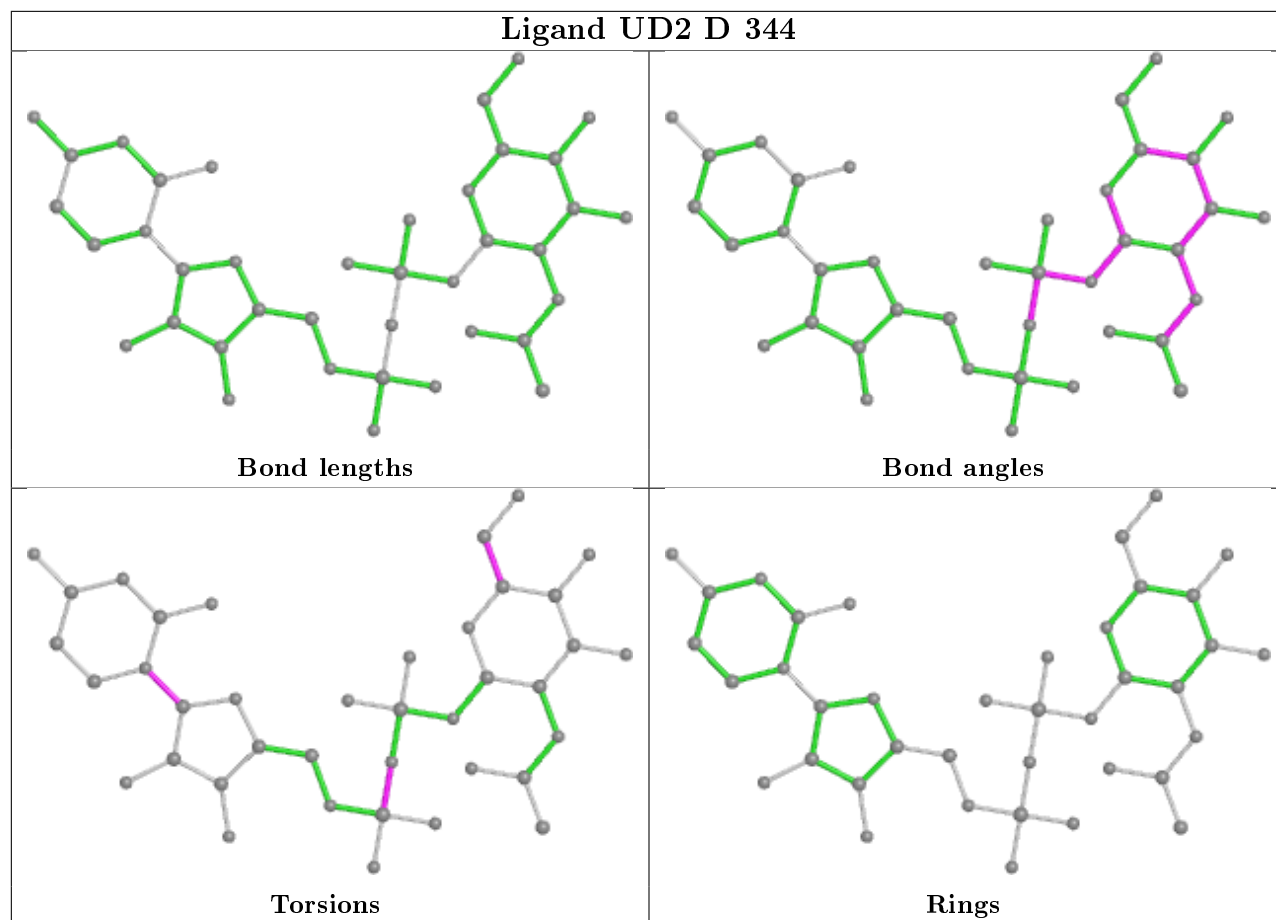
Mol	Chain	Res	Type	Atoms
2	A	343	NAD	C5D-O5D-PN-O2N
3	D	344	UD2	O5'-C5'-C6'-O6'
3	A	344	UD2	C1'-O1'-PB-O1B
2	A	343	NAD	O4B-C4B-C5B-O5B
3	C	344	UD2	C1'-O1'-PB-O3A
3	A	344	UD2	C1'-O1'-PB-O3A
2	D	343	NAD	C5D-O5D-PN-O3
2	B	343	NAD	C5D-O5D-PN-O3
2	C	343	NAD	O4B-C4B-C5B-O5B
2	D	343	NAD	O4B-C4B-C5B-O5B
2	B	343	NAD	O4B-C4B-C5B-O5B

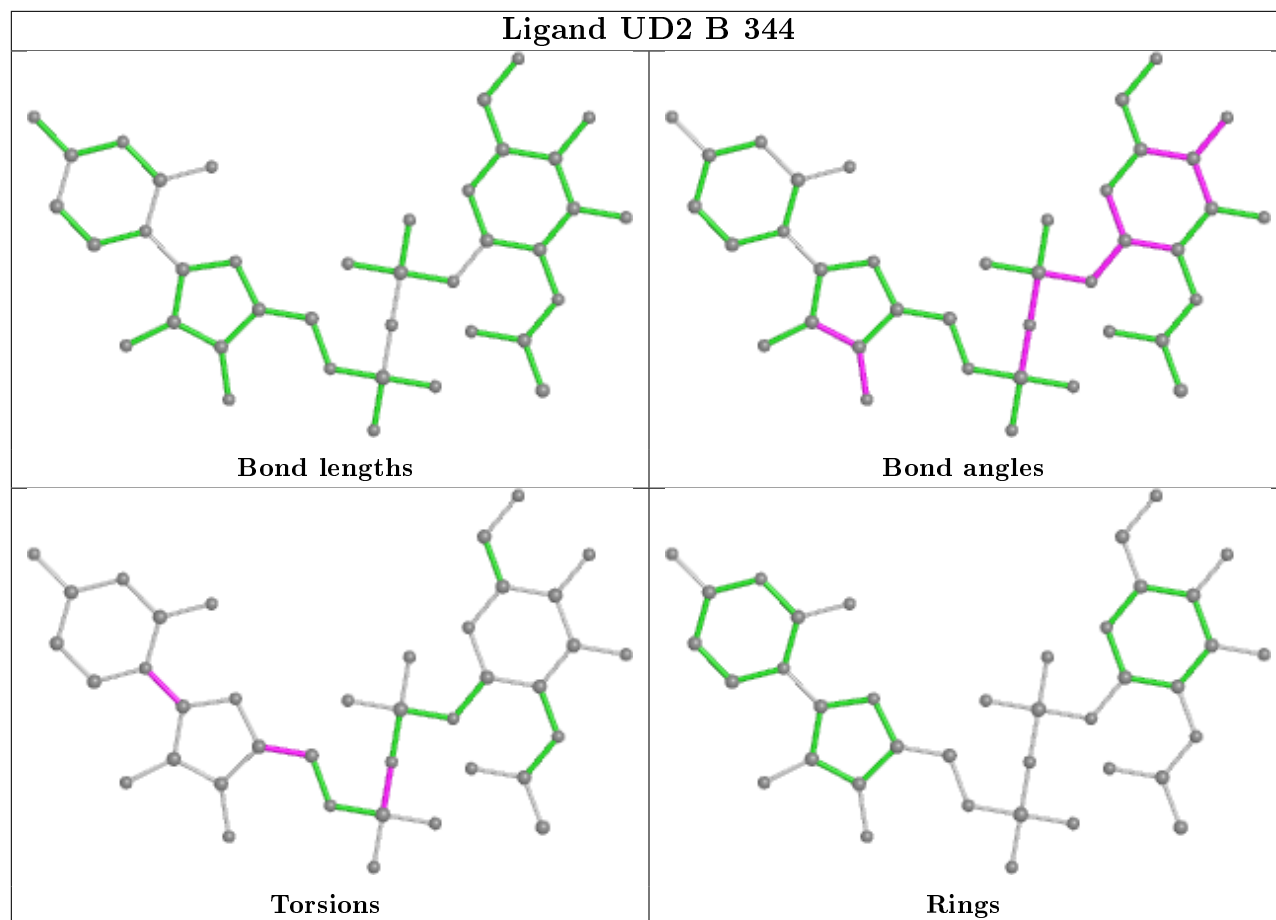
There are no ring outliers.

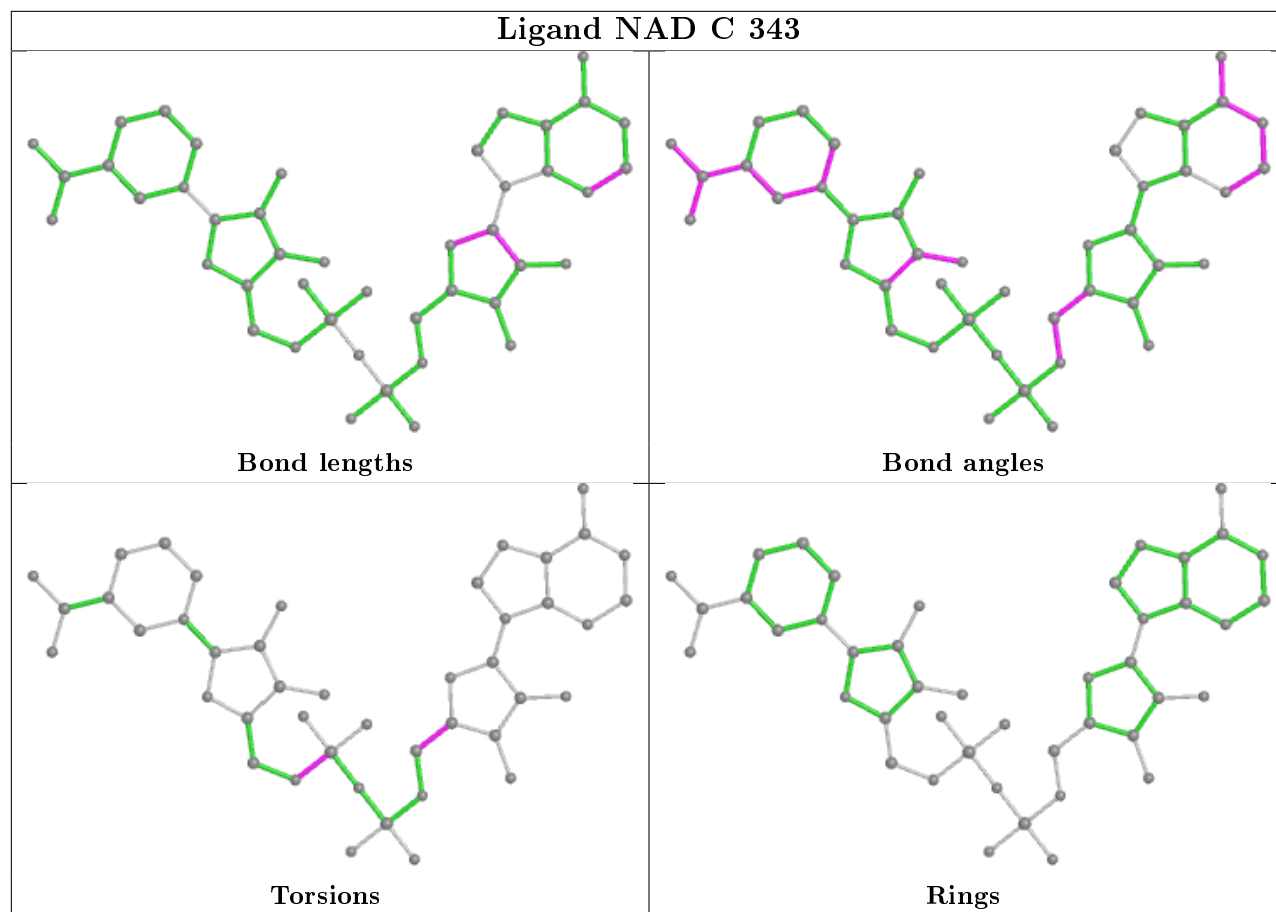
8 monomers are involved in 28 short contacts:

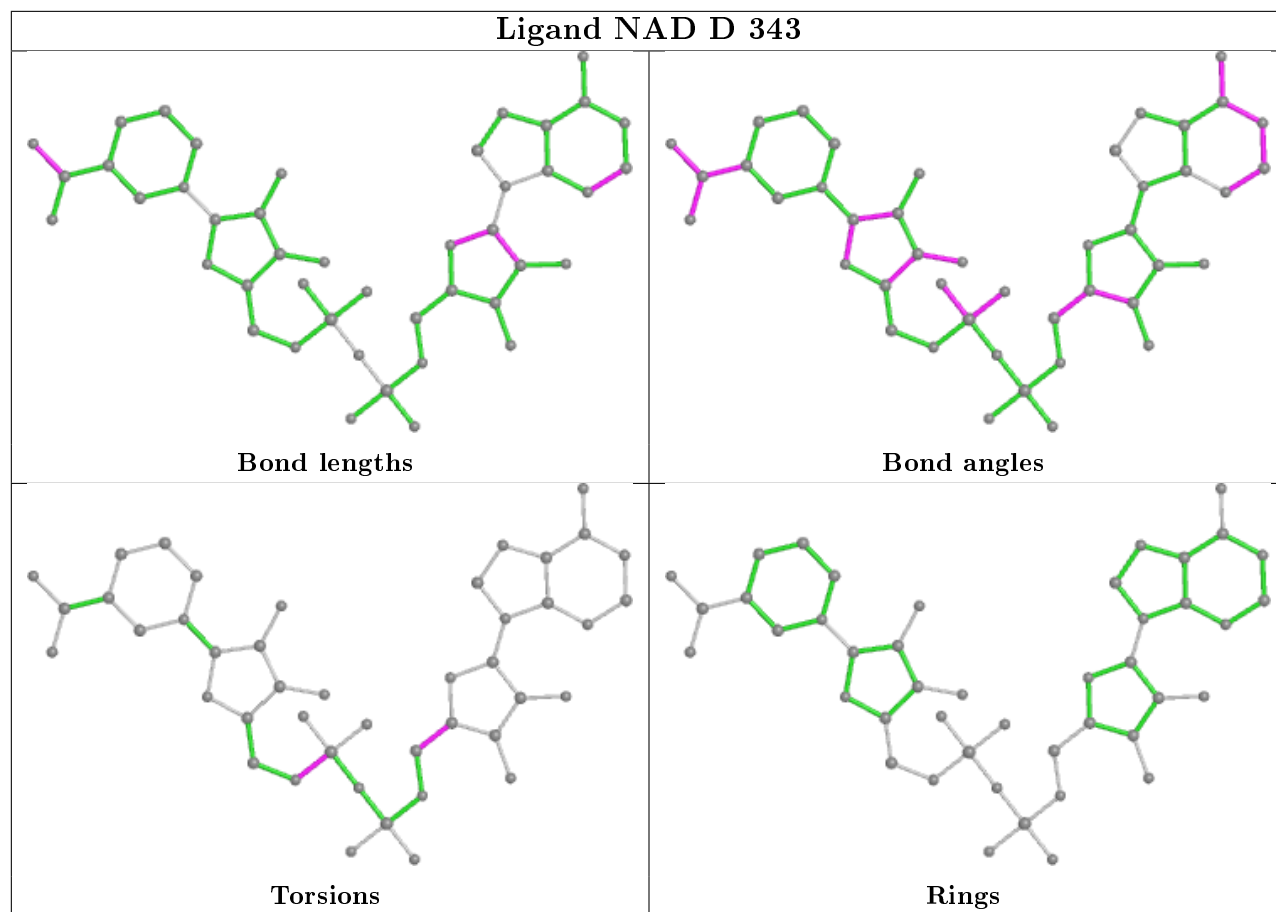
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	344	UD2	5	0
3	B	344	UD2	4	0
2	C	343	NAD	8	0
2	D	343	NAD	5	0
2	A	343	NAD	6	0
2	B	343	NAD	4	0
3	C	344	UD2	6	0
3	A	344	UD2	8	0

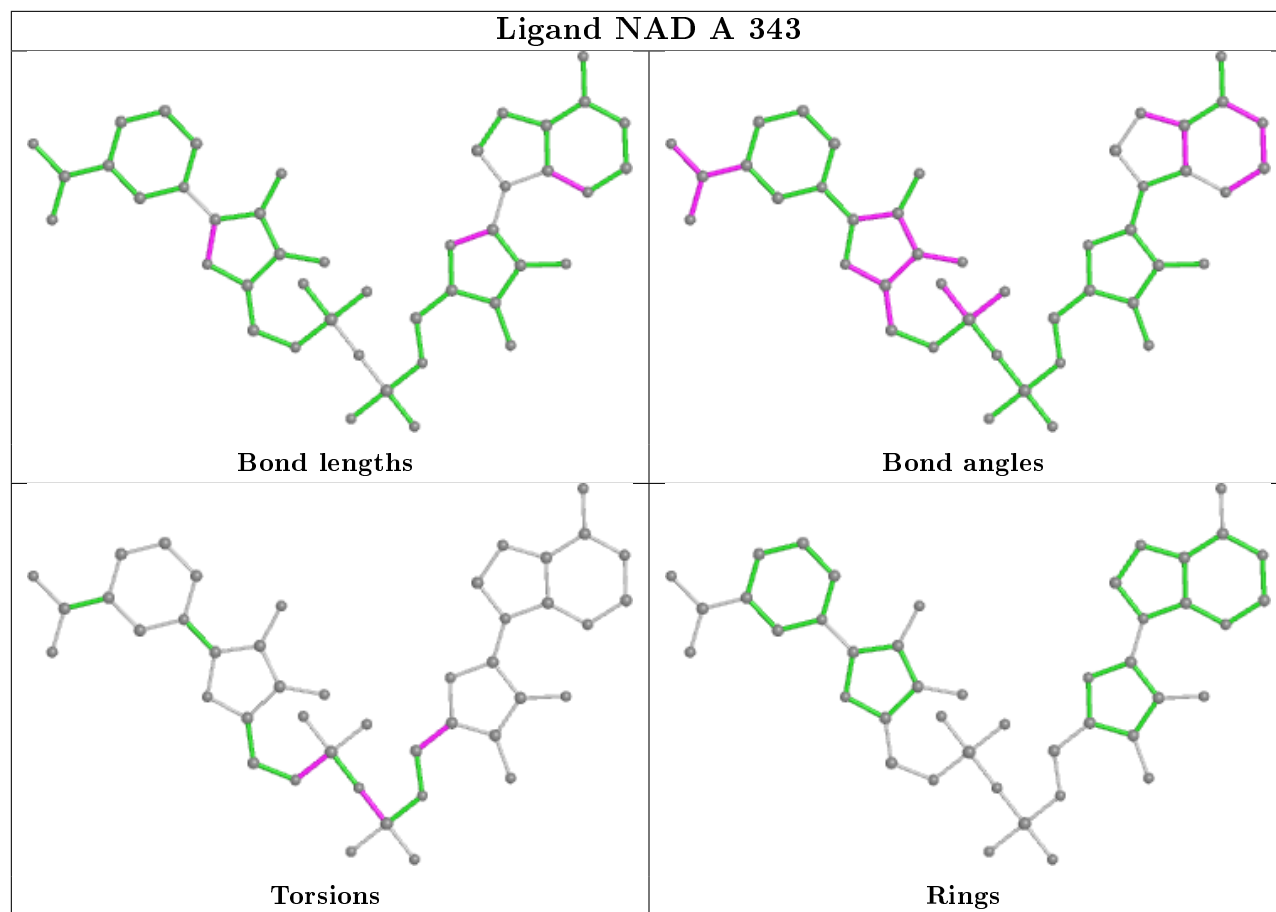
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

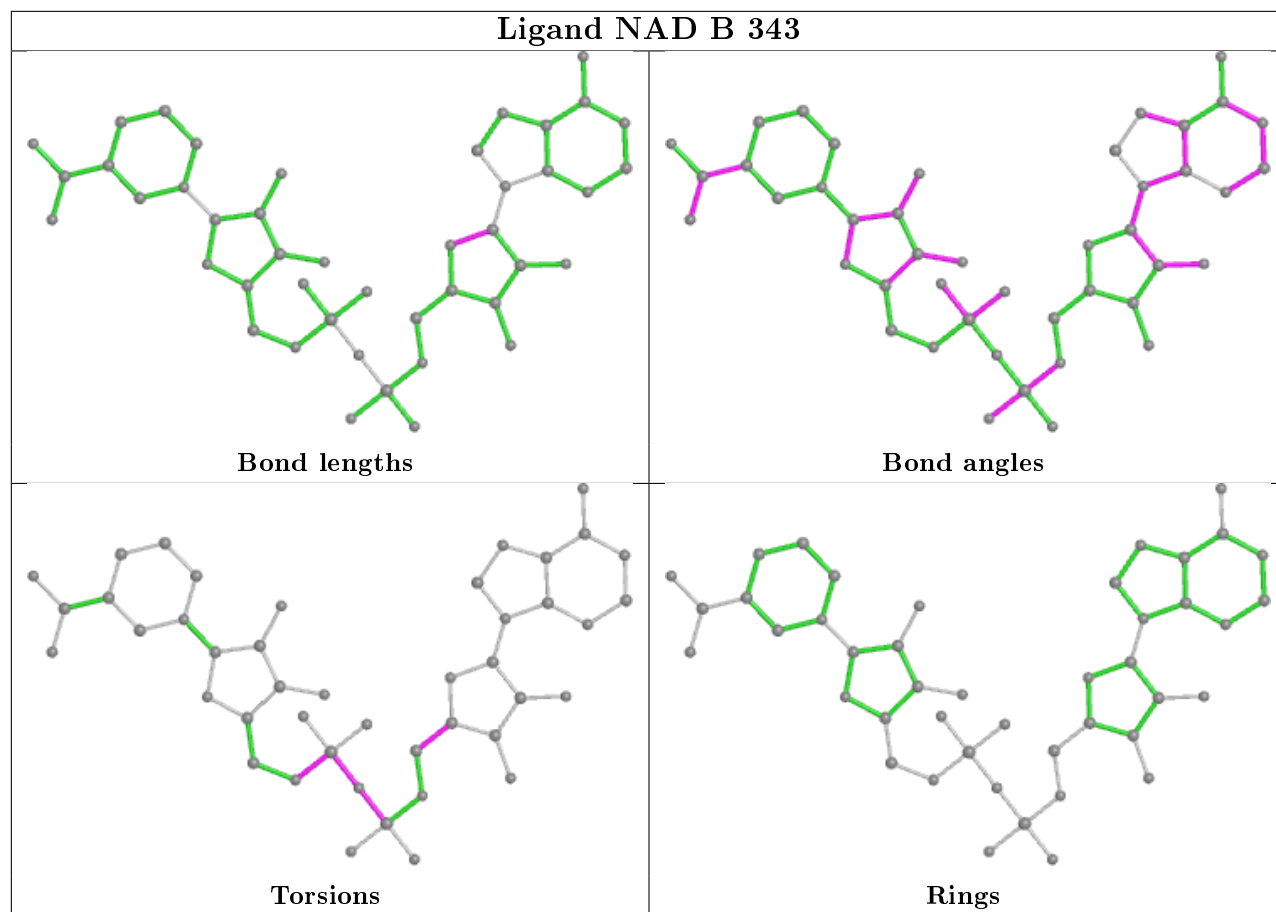


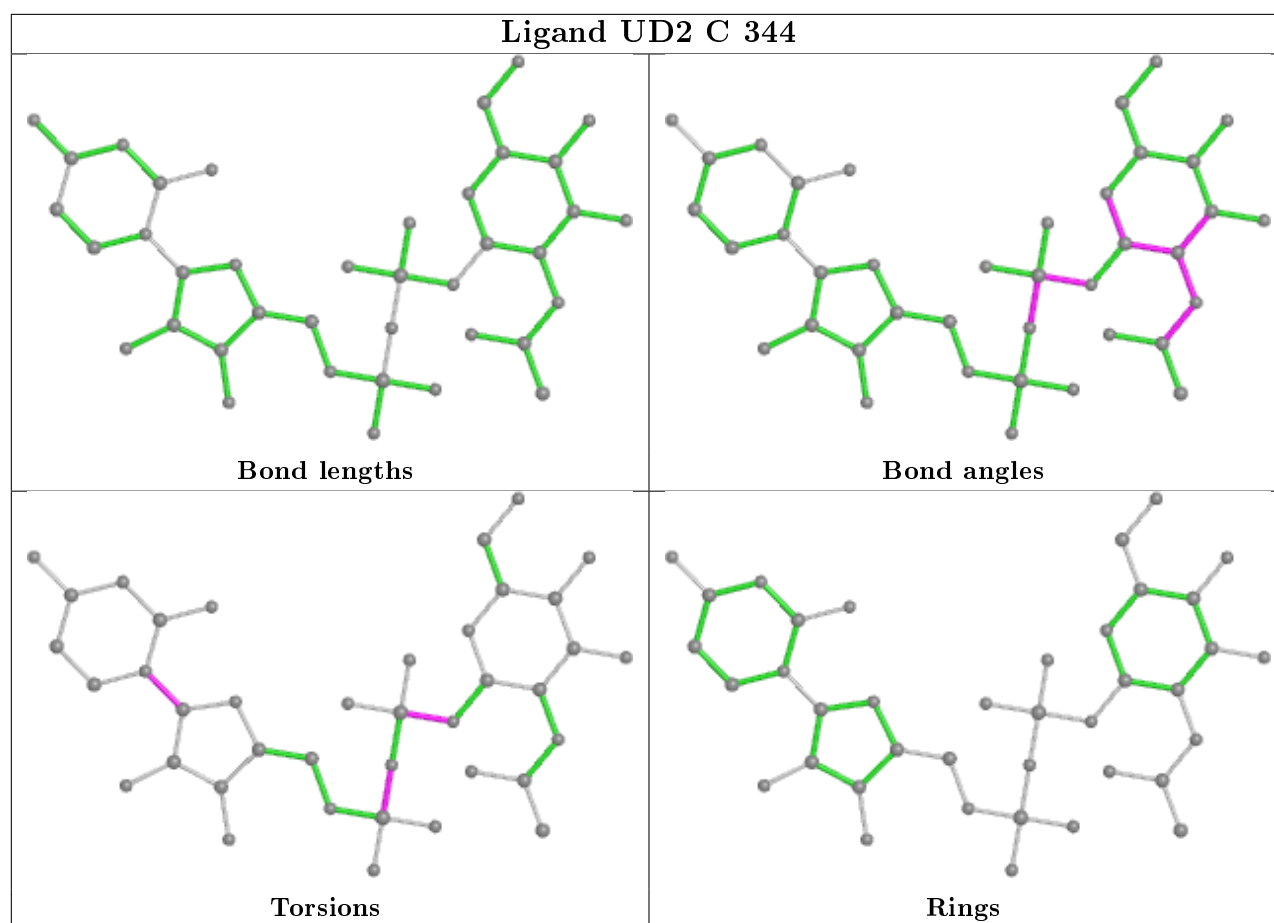


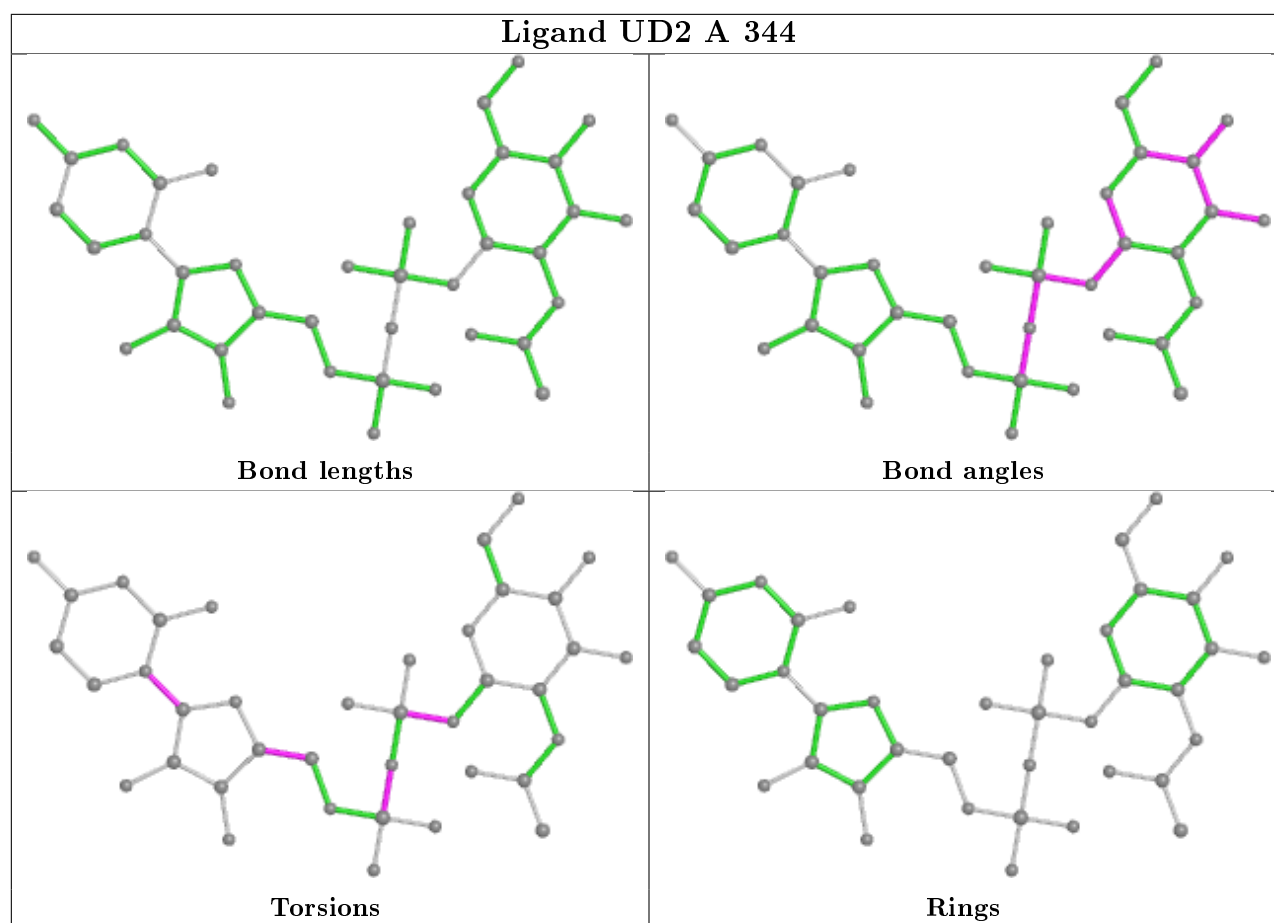












5.7 Other polymers [i](#)

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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	336/351 (95%)	0.44	9 (2%) 54 60	18, 29, 54, 85	0
1	B	336/351 (95%)	0.42	10 (2%) 50 56	18, 29, 54, 86	0
1	C	336/351 (95%)	0.40	11 (3%) 46 53	18, 30, 46, 68	0
1	D	336/351 (95%)	0.38	9 (2%) 54 60	19, 29, 45, 65	0
All	All	1344/1404 (95%)	0.41	39 (2%) 51 57	18, 29, 50, 86	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	ILE	4.8
1	B	287	HIS	4.2
1	B	282	LEU	4.2
1	D	286	HIS	3.9
1	A	287	HIS	3.9
1	D	2	MET	3.8
1	B	293	ILE	3.8
1	C	57	LEU	3.5
1	C	286	HIS	3.3
1	C	1	TYR	3.2
1	C	11	GLN	3.1
1	A	217	ALA	3.0
1	D	285	ILE	2.9
1	B	225	TYR	2.9
1	C	340	LEU	2.9
1	C	2	MET	2.9
1	C	279	TYR	2.8
1	A	230	GLY	2.8
1	D	293	ILE	2.7
1	D	320	ARG	2.5
1	C	285	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	316	LEU	2.5
1	B	336	TYR	2.4
1	D	279	TYR	2.4
1	A	144	SER	2.4
1	B	220	LYS	2.3
1	B	329	LEU	2.3
1	B	341	LYS	2.3
1	D	1	TYR	2.2
1	B	163	LEU	2.2
1	A	207	TYR	2.2
1	C	28	ILE	2.2
1	B	294	LYS	2.2
1	C	199	ARG	2.1
1	A	283	ASN	2.1
1	A	224	VAL	2.0
1	C	326	ARG	2.0
1	D	87	GLN	2.0
1	A	24	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	UD2	D	344	39/39	0.91	0.14	18,28,32,34	14
3	UD2	C	344	39/39	0.92	0.16	21,28,36,38	14
2	NAD	D	343	44/44	0.93	0.13	19,26,40,43	0
3	UD2	A	344	39/39	0.93	0.15	18,33,42,43	14
2	NAD	B	343	44/44	0.94	0.13	16,24,41,49	0

Continued on next page...

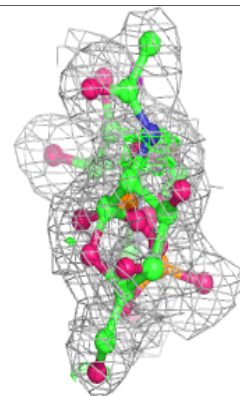
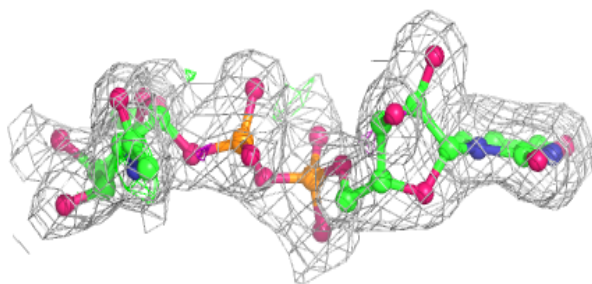
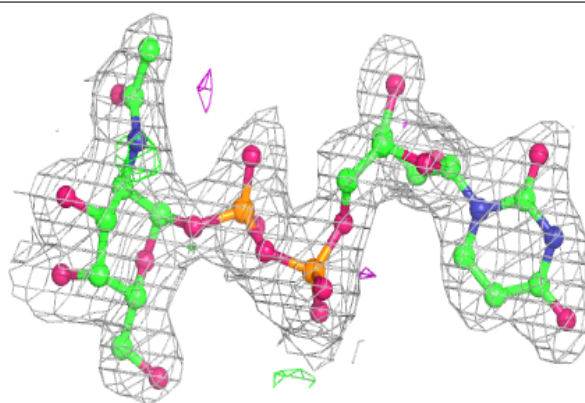
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAD	C	343	44/44	0.94	0.13	18,26,40,43	0
3	UD2	B	344	39/39	0.94	0.14	20,35,43,45	14
2	NAD	A	343	44/44	0.95	0.14	16,25,45,50	0
4	SO4	A	345	5/5	0.97	0.12	28,31,33,34	0
4	SO4	B	345	5/5	0.97	0.12	26,27,28,29	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.

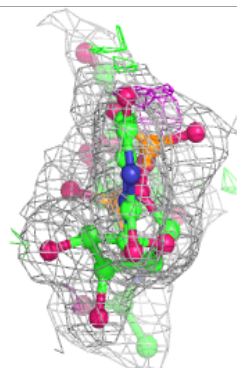
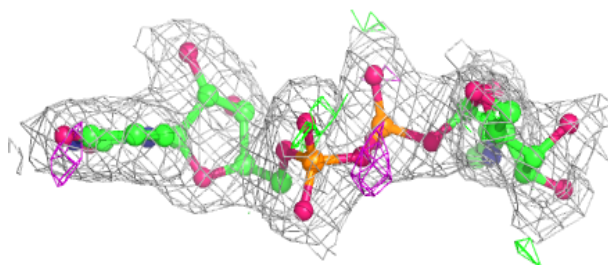
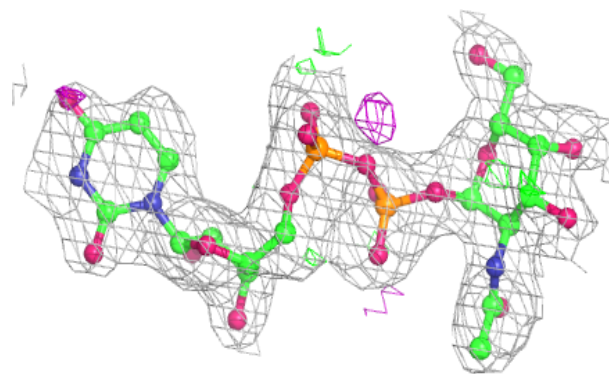
Electron density around UD2 D 344:

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

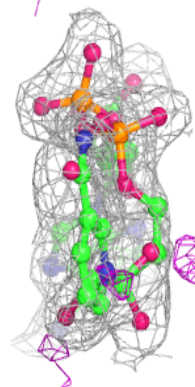
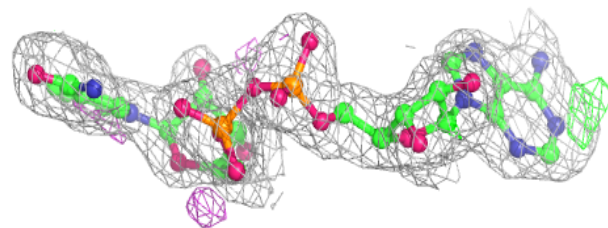
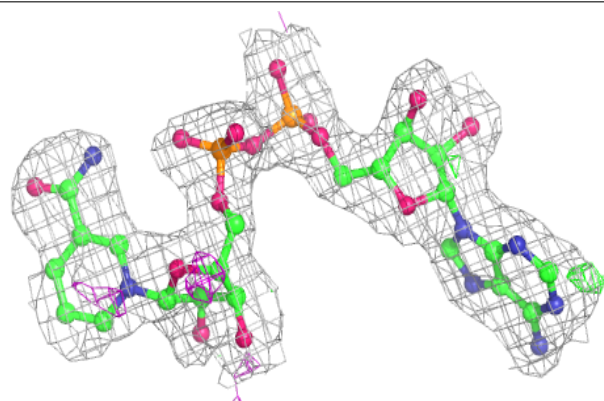


Electron density around UD2 C 344:

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

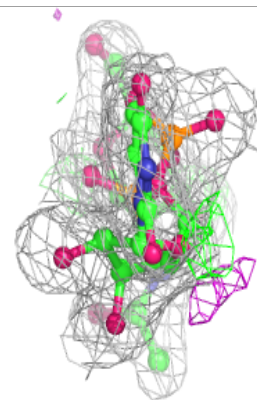
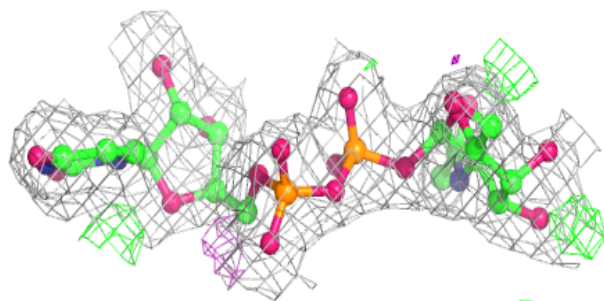
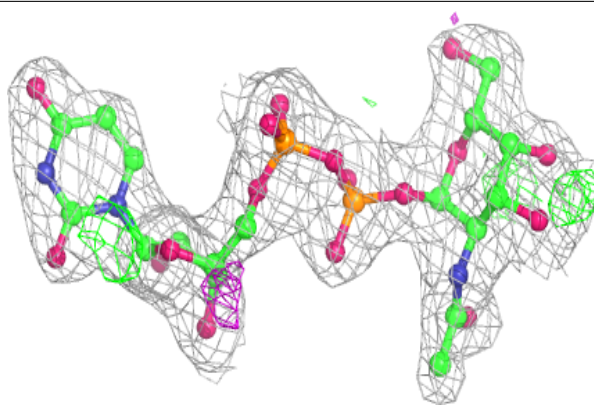
**Electron density around NAD D 343:**

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

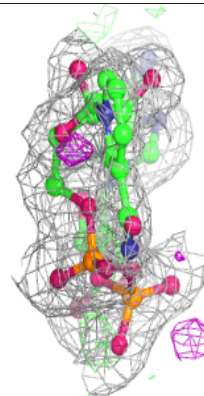
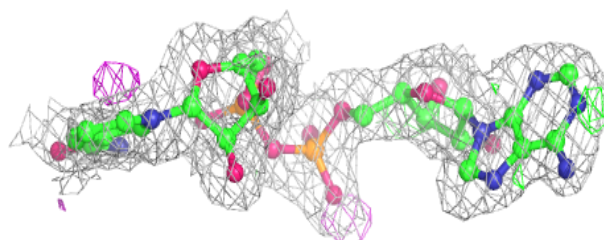
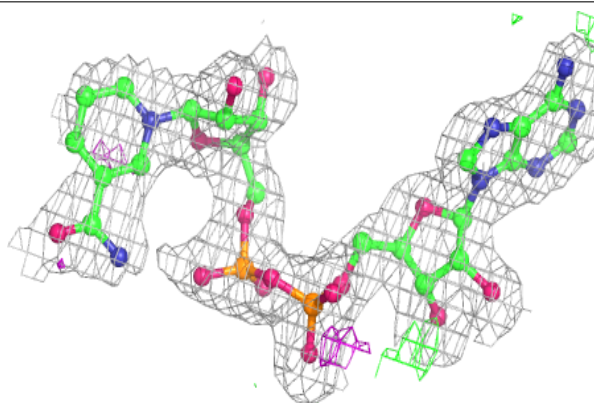


Electron density around UD2 A 344:

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

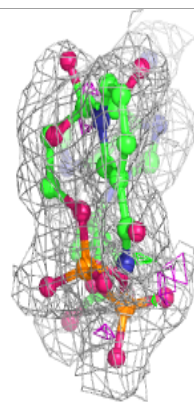
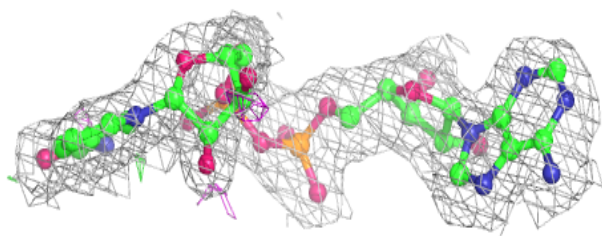
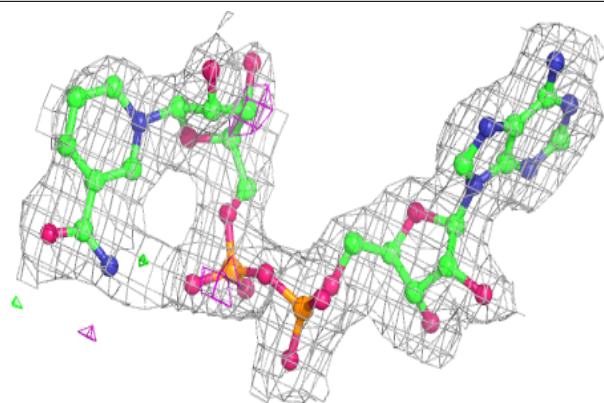
**Electron density around NAD B 343:**

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

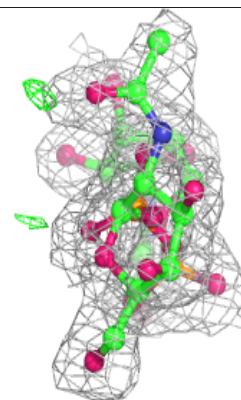
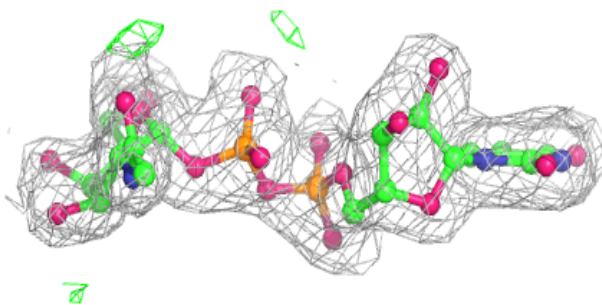
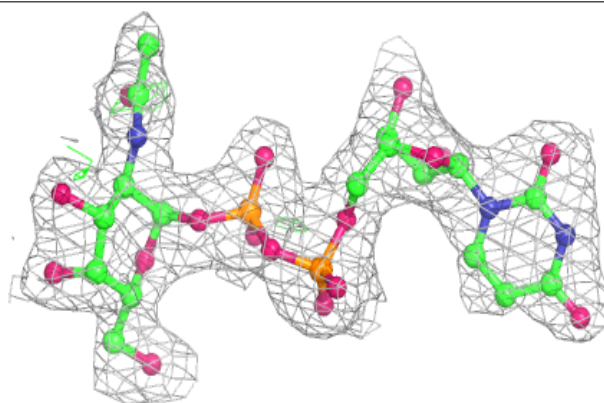


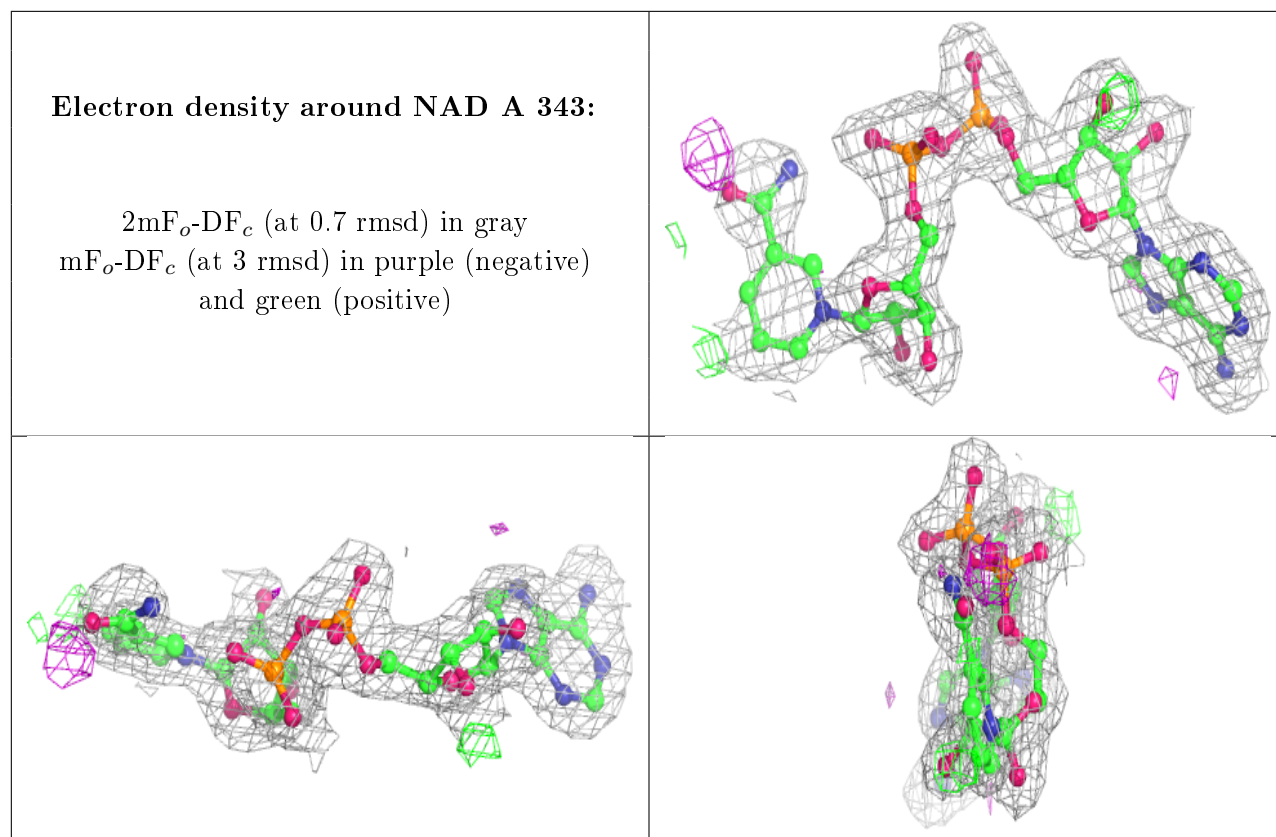
Electron density around NAD C 343:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.