



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:01 AM UTC

PDB ID : 3RUA / pdb_00003rua
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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

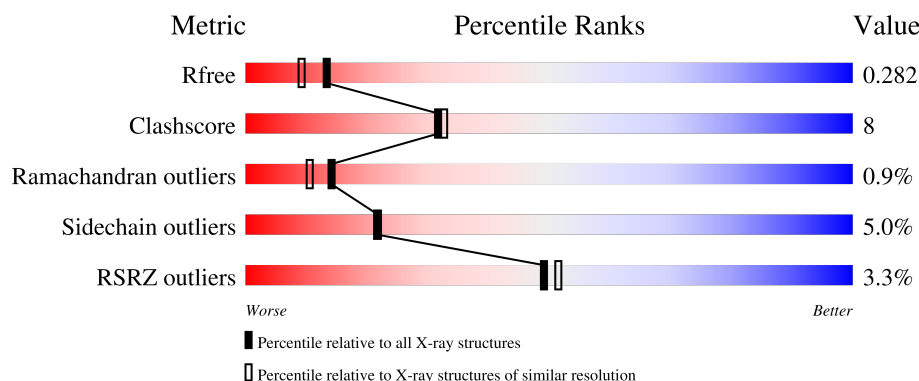
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	7% 76% 15% ...
1	B	351	5% 76% 16% ...
1	C	351	78% 16% ...
1	D	351	82% 12% ...

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11365 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:

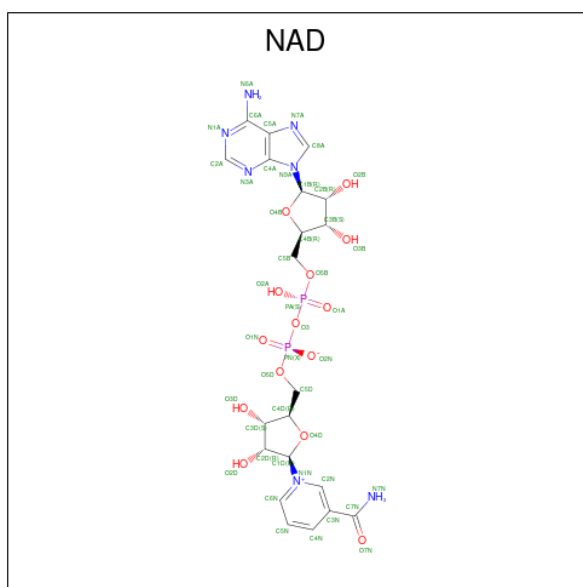
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	expression tag	UNP Q7BJX9
A	-7	HIS	-	expression tag	UNP Q7BJX9
A	-6	HIS	-	expression tag	UNP Q7BJX9
A	-5	HIS	-	expression tag	UNP Q7BJX9
A	-4	HIS	-	expression tag	UNP Q7BJX9
A	-3	HIS	-	expression tag	UNP Q7BJX9
B	-8	HIS	-	expression tag	UNP Q7BJX9
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 (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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 UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

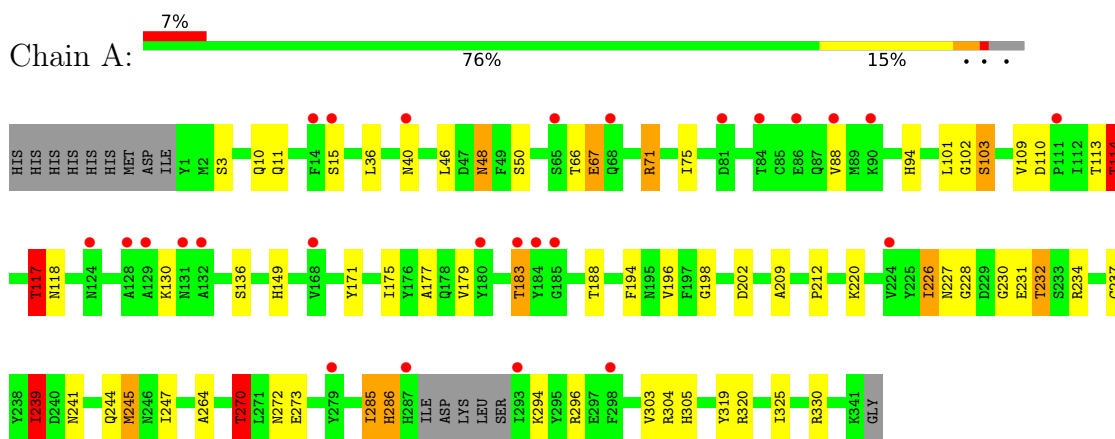
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	72	Total	O	0	0
			72	72		
5	C	106	Total	O	0	0
			106	106		
5	D	58	Total	O	0	0
			58	58		

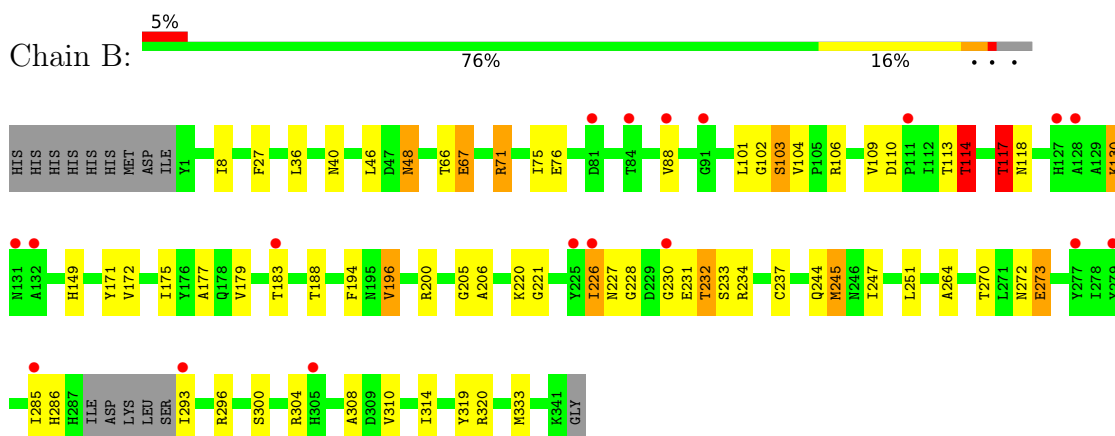
3 Residue-property plots [i](#)

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.

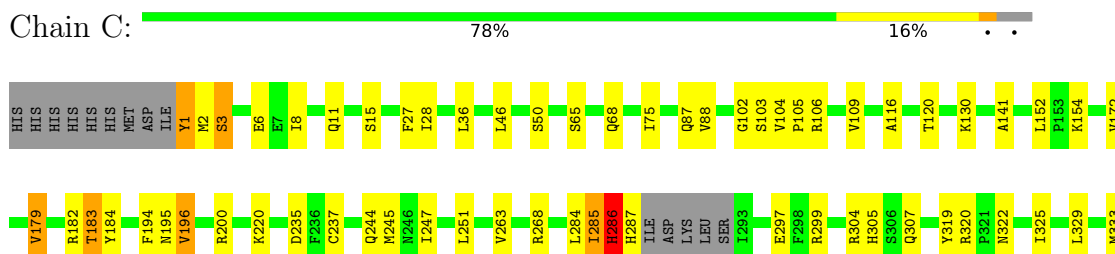
• Molecule 1: WbgU



• Molecule 1: WbgU

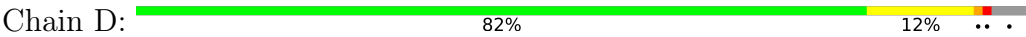


• Molecule 1: WbgU





● Molecule 1: WbgU



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	77.44Å 77.44Å 224.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.10) 99.9 (50.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.180 , 0.234 0.255 , 0.282	Depositor DCC
R_{free} test set	4402 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.477 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11365	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: NAD, UNL, SO4

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	1.28	4/2739 (0.1%)	1.19	14/3717 (0.4%)
1	B	1.26	3/2739 (0.1%)	1.18	9/3717 (0.2%)
1	C	1.19	3/2739 (0.1%)	1.11	4/3717 (0.1%)
1	D	1.17	0/2739	1.13	5/3717 (0.1%)
All	All	1.22	10/10956 (0.1%)	1.15	32/14868 (0.2%)

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	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	THR	CA-CB	7.63	1.65	1.53
1	C	109	VAL	CA-CB	7.29	1.63	1.54
1	A	117	THR	CB-CG2	-7.08	1.29	1.52
1	B	114	THR	CA-CB	7.01	1.64	1.53
1	C	325	ILE	CA-CB	6.66	1.61	1.54
1	B	117	THR	CB-CG2	-5.44	1.34	1.52
1	C	247	ILE	CA-CB	5.17	1.61	1.54
1	A	270	THR	CA-CB	5.13	1.61	1.53
1	B	104	VAL	CA-C	5.13	1.58	1.52
1	A	303	VAL	CA-CB	5.06	1.59	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	239	ILE	CB-CA-C	-11.83	96.54	112.04
1	A	239	ILE	CB-CA-C	-9.06	98.11	112.16
1	C	3	SER	N-CA-C	8.86	120.71	111.14
1	B	200	ARG	NE-CZ-NH2	-8.75	111.32	119.20
1	D	3	SER	N-CA-C	7.62	121.06	111.69
1	A	239	ILE	CG1-CB-CG2	7.26	132.47	110.70
1	B	149	HIS	CA-C-N	-6.24	113.52	120.45
1	B	149	HIS	C-N-CA	-6.24	113.52	120.45
1	C	200	ARG	NE-CZ-NH2	-6.18	113.64	119.20
1	A	245	MET	CG-SD-CE	-6.04	87.61	100.90
1	A	3	SER	N-CA-C	5.97	118.30	111.02
1	A	149	HIS	CA-C-N	-5.92	113.88	120.45
1	A	149	HIS	C-N-CA	-5.92	113.88	120.45
1	B	245	MET	CG-SD-CE	-5.90	87.92	100.90
1	B	232	THR	CB-CA-C	5.81	118.80	109.61
1	A	232	THR	CB-CA-C	5.68	118.85	109.70
1	C	299	ARG	N-CA-C	-5.64	102.05	110.23
1	D	36	LEU	N-CA-C	5.64	117.42	111.28
1	D	245	MET	CG-SD-CE	-5.45	88.92	100.90
1	A	15	SER	CA-C-N	-5.42	114.37	119.85
1	A	15	SER	C-N-CA	-5.42	114.37	119.85
1	A	113	THR	CA-C-N	5.21	127.25	120.28
1	A	113	THR	C-N-CA	5.21	127.25	120.28
1	A	286	HIS	N-CA-C	5.16	121.78	110.80
1	C	36	LEU	N-CA-C	5.15	116.89	111.28
1	B	200	ARG	NE-CZ-NH1	5.13	126.63	121.50
1	B	221	GLY	N-CA-C	-5.12	106.05	114.76
1	B	113	THR	CA-C-N	5.11	127.13	120.28
1	B	113	THR	C-N-CA	5.11	127.13	120.28
1	D	210	VAL	N-CA-C	5.07	115.29	110.42
1	A	202	ASP	CA-C-N	-5.01	114.98	121.04
1	A	202	ASP	C-N-CA	-5.01	114.98	121.04

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	ILE	Peptide
1	C	285	ILE	Peptide
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	2681	0	2658	51	0
1	B	2681	0	2658	60	0
1	C	2681	0	2658	41	0
1	D	2681	0	2658	35	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
3	C	25	0	0	0	0
3	D	25	0	0	0	0
4	A	10	0	0	0	0
5	A	119	0	0	0	0
5	B	72	0	0	0	0
5	C	106	0	0	2	0
5	D	58	0	0	0	0
All	All	11365	0	10736	177	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 (177) 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:286:HIS:O	1:C:287:HIS:ND1	1.88	1.05
1:C:2:MET:HG3	1:C:322:ASN:HD21	1.25	1.01
1:D:2:MET:HG2	1:D:322:ASN:HD21	1.24	0.99
1:C:2:MET:CG	1:C:322:ASN:HD21	1.75	0.99
1:A:171:TYR:CE2	1:A:175:ILE:HD11	2.02	0.94
1:D:75:ILE:HD13	1:D:88:VAL:HG12	1.55	0.88
1:D:2:MET:CG	1:D:322:ASN:HD21	1.87	0.87
1:B:40:ASN:HB3	1:B:71:ARG:HH22	1.41	0.85
1:D:245:MET:HE1	1:D:319:TYR:CD1	2.12	0.83
1:C:179:VAL:O	1:C:183:THR:HG23	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:VAL:O	1:D:183:THR:HG23	1.78	0.82
1:A:270:THR:OG1	1:A:273:GLU:HG3	1.79	0.82
1:A:67:GLU:H	1:A:67:GLU:CD	1.90	0.79
1:D:286:HIS:O	1:D:287:HIS:ND1	2.14	0.79
1:C:2:MET:HG3	1:C:322:ASN:ND2	1.98	0.79
1:B:171:TYR:CE2	1:B:175:ILE:HD11	2.17	0.79
1:A:171:TYR:CZ	1:A:175:ILE:HD11	2.19	0.78
1:B:244:GLN:HE22	1:B:320:ARG:H	1.31	0.78
1:B:40:ASN:HB3	1:B:71:ARG:NH2	1.98	0.77
1:D:2:MET:HG2	1:D:322:ASN:ND2	1.99	0.77
1:A:40:ASN:HB3	1:A:71:ARG:HH22	1.50	0.77
1:B:270:THR:OG1	1:B:273:GLU:HG3	1.85	0.76
1:B:67:GLU:H	1:B:67:GLU:CD	1.93	0.76
1:D:286:HIS:O	1:D:287:HIS:CG	2.39	0.76
1:B:232:THR:HG23	1:B:304:ARG:O	1.87	0.74
1:A:230:GLY:O	1:A:272:ASN:ND2	2.21	0.74
1:A:232:THR:HG23	1:A:304:ARG:O	1.88	0.73
1:A:117:THR:HG22	1:A:118:ASN:OD1	1.89	0.73
1:C:75:ILE:HD13	1:C:88:VAL:HG12	1.70	0.73
1:D:245:MET:HE1	1:D:319:TYR:CG	2.22	0.73
1:A:244:GLN:HE22	1:A:320:ARG:H	1.36	0.73
1:C:286:HIS:O	1:C:287:HIS:CG	2.41	0.73
1:B:66:THR:HB	1:B:67:GLU:OE2	1.90	0.71
1:C:27:PHE:HE2	1:C:196:VAL:HG23	1.55	0.71
1:C:245:MET:HE1	1:C:319:TYR:CG	2.26	0.70
1:C:244:GLN:HE22	1:C:320:ARG:H	1.39	0.69
1:B:232:THR:HG22	1:B:234:ARG:HH12	1.58	0.69
1:A:75:ILE:HD13	1:A:88:VAL:HG12	1.74	0.69
1:D:280:ASP:O	1:D:284:LEU:HD13	1.94	0.68
1:A:101:LEU:HG	1:A:117:THR:HG21	1.77	0.67
1:A:66:THR:HB	1:A:67:GLU:OE2	1.94	0.67
1:C:102:GLY:O	1:C:103:SER:HB3	1.94	0.66
1:B:270:THR:OG1	1:B:273:GLU:CG	2.43	0.66
1:C:27:PHE:CE2	1:C:196:VAL:HG23	2.31	0.66
1:D:8:ILE:HG23	1:D:251:LEU:HD22	1.76	0.65
1:A:40:ASN:HB3	1:A:71:ARG:NH2	2.12	0.65
1:B:230:GLY:O	1:B:272:ASN:ND2	2.30	0.65
1:B:75:ILE:HD13	1:B:88:VAL:HG12	1.78	0.65
1:A:10:GLN:HE21	1:B:106:ARG:HH11	1.45	0.65
1:B:232:THR:HG22	1:B:234:ARG:NH1	2.11	0.64
1:B:244:GLN:NE2	1:B:320:ARG:H	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:MET:HE1	1:B:319:TYR:CD2	2.33	0.63
1:B:245:MET:HE1	1:B:319:TYR:CG	2.34	0.63
1:A:244:GLN:NE2	1:A:320:ARG:H	1.95	0.63
1:A:245:MET:HE1	1:A:319:TYR:CD2	2.33	0.63
1:A:94:HIS:HD2	1:A:136:SER:OG	1.81	0.63
1:C:245:MET:HG2	1:C:263:VAL:HG22	1.82	0.62
1:B:228:GLY:N	1:B:296:ARG:O	2.31	0.62
1:A:232:THR:HG22	1:A:234:ARG:HH12	1.65	0.61
1:A:40:ASN:O	1:A:71:ARG:NH2	2.33	0.60
1:A:270:THR:OG1	1:A:273:GLU:CG	2.49	0.60
1:D:75:ILE:HD13	1:D:88:VAL:CG1	2.29	0.59
1:C:65:SER:H	1:C:68:GLN:HE21	1.50	0.59
1:A:230:GLY:C	1:A:272:ASN:HD21	2.10	0.59
1:B:67:GLU:CD	1:B:67:GLU:N	2.60	0.59
1:B:117:THR:HG22	1:B:118:ASN:OD1	2.01	0.59
1:D:245:MET:CE	1:D:319:TYR:CD1	2.84	0.59
1:B:102:GLY:O	1:B:103:SER:HB3	2.03	0.58
1:A:245:MET:HE1	1:A:319:TYR:CG	2.39	0.58
1:B:270:THR:N	1:B:273:GLU:OE1	2.31	0.57
1:C:244:GLN:NE2	1:C:320:ARG:H	2.02	0.57
1:A:67:GLU:CD	1:A:67:GLU:N	2.60	0.57
1:B:232:THR:CG2	1:B:234:ARG:HH12	2.18	0.57
1:B:27:PHE:HE2	1:B:196:VAL:CG2	2.17	0.56
1:D:102:GLY:O	1:D:103:SER:HB3	2.04	0.56
1:A:232:THR:HG22	1:A:234:ARG:NH1	2.20	0.56
1:C:2:MET:CG	1:C:322:ASN:ND2	2.58	0.56
1:C:285:ILE:O	1:C:285:ILE:HG22	2.04	0.56
1:B:27:PHE:HE2	1:B:196:VAL:HG22	1.70	0.55
1:A:231:GLU:OE2	1:A:231:GLU:HA	2.07	0.55
1:A:102:GLY:O	1:A:103:SER:HB3	2.05	0.55
1:D:245:MET:HE1	1:D:319:TYR:CE1	2.43	0.54
1:C:154:LYS:HD3	5:C:423:HOH:O	2.07	0.54
1:A:10:GLN:NE2	1:B:106:ARG:HH11	2.05	0.53
1:B:226:ILE:HG22	1:B:226:ILE:O	2.08	0.53
1:A:232:THR:CG2	1:A:234:ARG:HH12	2.21	0.53
1:A:36:LEU:HD21	1:A:247:ILE:HD11	1.89	0.53
1:C:8:ILE:HG23	1:C:251:LEU:HD22	1.90	0.53
1:B:27:PHE:CE2	1:B:196:VAL:CG2	2.93	0.52
1:B:304:ARG:O	1:B:304:ARG:HD2	2.10	0.52
1:A:179:VAL:O	1:A:183:THR:HG23	2.11	0.51
1:D:304:ARG:HG3	1:D:305:HIS:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ASP:HB2	1:D:307:GLN:HA	1.93	0.51
1:B:231:GLU:O	1:B:232:THR:C	2.53	0.50
1:D:245:MET:HG2	1:D:263:VAL:HG22	1.93	0.50
1:C:333:MET:HA	1:C:333:MET:HE2	1.92	0.50
1:D:196:VAL:HA	1:D:237:CYS:O	2.11	0.50
1:D:179:VAL:O	1:D:183:THR:CG2	2.55	0.50
1:A:11:GLN:NE2	1:B:206:ALA:H	2.10	0.49
1:C:235:ASP:HB2	1:C:307:GLN:HA	1.95	0.49
1:B:40:ASN:O	1:B:71:ARG:NH2	2.36	0.49
1:B:231:GLU:OE2	1:B:231:GLU:HA	2.13	0.49
1:C:104:VAL:HB	1:C:105:PRO:HD3	1.94	0.49
1:A:110:ASP:O	1:A:114:THR:HB	2.12	0.49
1:C:245:MET:HE1	1:C:319:TYR:CD1	2.48	0.48
1:C:194:PHE:O	1:C:195:ASN:C	2.56	0.48
1:B:230:GLY:C	1:B:272:ASN:HD21	2.22	0.48
1:A:230:GLY:C	1:A:272:ASN:ND2	2.70	0.47
1:C:245:MET:HE1	1:C:319:TYR:CD2	2.48	0.47
1:B:8:ILE:HG23	1:B:251:LEU:HD22	1.95	0.47
1:C:245:MET:CE	1:C:319:TYR:CD1	2.98	0.47
1:C:2:MET:HG2	1:C:322:ASN:HD21	1.71	0.47
1:D:198:GLY:HA3	1:D:239:ILE:CD1	2.44	0.47
1:B:130:LYS:NZ	1:D:67:GLU:OE1	2.38	0.47
1:B:314:ILE:HG23	1:B:320:ARG:NH1	2.30	0.47
1:C:65:SER:H	1:C:68:GLN:NE2	2.13	0.47
1:A:177:ALA:HB1	1:A:188:THR:OG1	2.15	0.47
1:D:245:MET:CE	1:D:319:TYR:CE1	2.99	0.46
1:A:11:GLN:HE21	1:B:206:ALA:H	1.62	0.46
1:B:233:SER:O	1:B:234:ARG:HD3	2.16	0.46
1:A:209:ALA:O	1:A:212:PRO:HD2	2.16	0.46
1:C:130:LYS:HD2	1:C:184:TYR:CG	2.51	0.46
1:A:320:ARG:HH21	1:B:76:GLU:CD	2.24	0.46
1:B:310:VAL:O	1:B:314:ILE:HG13	2.15	0.46
1:D:104:VAL:HB	1:D:105:PRO:HD3	1.98	0.46
1:B:177:ALA:HB1	1:B:188:THR:OG1	2.16	0.45
1:D:245:MET:HB2	1:D:245:MET:HE2	1.42	0.45
1:A:196:VAL:HA	1:A:237:CYS:O	2.17	0.45
1:C:50:SER:HB2	1:D:14:PHE:CG	2.51	0.45
1:C:1:TYR:HA	1:C:6:GLU:OE2	2.17	0.45
1:D:116:ALA:O	1:D:120:THR:HB	2.17	0.44
1:B:304:ARG:HD2	1:B:304:ARG:C	2.42	0.44
1:A:11:GLN:HE22	1:B:205:GLY:HA2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:TYR:CZ	1:B:175:ILE:HD11	2.50	0.44
1:A:94:HIS:CD2	1:A:136:SER:OG	2.67	0.44
1:B:333:MET:HE2	1:B:333:MET:HA	2.00	0.44
1:D:225:TYR:HB3	1:D:296:ARG:HE	1.82	0.44
1:B:101:LEU:HG	1:B:117:THR:HG21	2.00	0.44
1:B:245:MET:HB2	1:B:245:MET:HE2	1.49	0.44
1:B:36:LEU:HD21	1:B:247:ILE:HD11	1.99	0.43
1:A:228:GLY:N	1:A:296:ARG:O	2.48	0.43
1:C:2:MET:N	1:C:6:GLU:OE2	2.51	0.43
1:D:2:MET:N	1:D:6:GLU:OE2	2.52	0.43
1:D:194:PHE:O	1:D:195:ASN:C	2.59	0.43
1:B:231:GLU:O	1:B:270:THR:HG22	2.19	0.43
1:C:329:LEU:O	1:C:333:MET:HG2	2.19	0.43
1:A:36:LEU:HD21	1:A:247:ILE:CD1	2.49	0.43
1:A:294:LYS:HE2	1:A:294:LYS:HB3	1.71	0.43
1:B:110:ASP:O	1:B:114:THR:HB	2.19	0.43
1:C:141:ALA:HB1	5:C:383:HOH:O	2.17	0.43
1:A:194:PHE:HB2	1:A:264:ALA:HB2	2.00	0.42
1:C:196:VAL:HA	1:C:237:CYS:O	2.19	0.42
1:B:48:ASN:HD22	1:B:48:ASN:H	1.66	0.42
1:D:130:LYS:HD2	1:D:184:TYR:CG	2.54	0.42
1:B:179:VAL:O	1:B:183:THR:HG23	2.20	0.42
1:D:285:ILE:O	1:D:285:ILE:HG22	2.19	0.42
1:A:241:ASN:HB3	1:A:319:TYR:OH	2.20	0.42
1:A:48:ASN:HD22	1:A:48:ASN:H	1.68	0.42
1:B:172:VAL:HG22	1:C:172:VAL:HG22	2.01	0.42
1:A:270:THR:OG1	1:A:273:GLU:CD	2.63	0.41
1:B:36:LEU:HD21	1:B:247:ILE:CD1	2.50	0.41
1:B:264:ALA:HB3	1:B:308:ALA:HB3	2.01	0.41
1:B:196:VAL:HA	1:B:237:CYS:O	2.20	0.41
1:A:171:TYR:CE2	1:A:175:ILE:CD1	2.90	0.41
1:A:226:ILE:O	1:A:226:ILE:HG22	2.19	0.41
1:B:48:ASN:HD22	1:B:48:ASN:N	2.16	0.41
1:B:194:PHE:HB2	1:B:264:ALA:HB2	2.03	0.41
1:C:304:ARG:HG3	1:C:305:HIS:CD2	2.56	0.41
1:D:2:MET:HG3	1:D:322:ASN:HD21	1.80	0.41
1:A:245:MET:HE2	1:A:245:MET:HB2	1.64	0.41
1:B:228:GLY:CA	1:B:296:ARG:O	2.69	0.41
1:C:28:ILE:HD11	1:C:196:VAL:HG21	2.01	0.41
1:C:116:ALA:O	1:C:120:THR:HB	2.20	0.40
1:C:285:ILE:O	1:C:285:ILE:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:HIS:C	1:D:287:HIS:CG	2.99	0.40
1:A:198:GLY:HA3	1:A:239:ILE:HG12	2.02	0.40
1:C:106:ARG:NH1	1:D:14:PHE:O	2.47	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%)	319 (96%)	7 (2%)	6 (2%)	6	3
1	B	332/351 (95%)	313 (94%)	15 (4%)	4 (1%)	10	7
1	C	332/351 (95%)	324 (98%)	7 (2%)	1 (0%)	36	36
1	D	332/351 (95%)	322 (97%)	9 (3%)	1 (0%)	36	36
All	All	1328/1404 (95%)	1278 (96%)	38 (3%)	12 (1%)	14	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	286	HIS
1	B	227	ASN
1	C	286	HIS
1	D	286	HIS
1	B	286	HIS
1	A	50	SER
1	A	103	SER
1	A	226	ILE
1	B	103	SER
1	B	226	ILE
1	A	325	ILE

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%)	275 (95%)	15 (5%)	21	20
1	B	290/304 (95%)	276 (95%)	14 (5%)	23	23
1	C	290/304 (95%)	273 (94%)	17 (6%)	18	16
1	D	290/304 (95%)	278 (96%)	12 (4%)	27	29
All	All	1160/1216 (95%)	1102 (95%)	58 (5%)	22	22

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	48	ASN
1	A	67	GLU
1	A	71	ARG
1	A	109	VAL
1	A	114	THR
1	A	117	THR
1	A	130	LYS
1	A	183	THR
1	A	220	LYS
1	A	239	ILE
1	A	270	THR
1	A	285	ILE
1	A	305	HIS
1	A	330	ARG
1	B	46	LEU
1	B	48	ASN
1	B	67	GLU
1	B	71	ARG
1	B	109	VAL
1	B	114	THR
1	B	117	THR
1	B	130	LYS
1	B	196	VAL

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Mol	Chain	Res	Type
1	B	220	LYS
1	B	273	GLU
1	B	285	ILE
1	B	293	ILE
1	B	300	SER
1	C	1	TYR
1	C	3	SER
1	C	11	GLN
1	C	15	SER
1	C	46	LEU
1	C	87	GLN
1	C	152	LEU
1	C	179	VAL
1	C	182	ARG
1	C	183	THR
1	C	196	VAL
1	C	220	LYS
1	C	268	ARG
1	C	284	LEU
1	C	286	HIS
1	C	297	GLU
1	C	338	ARG
1	D	3	SER
1	D	15	SER
1	D	46	LEU
1	D	152	LEU
1	D	179	VAL
1	D	183	THR
1	D	220	LYS
1	D	239	ILE
1	D	260	ILE
1	D	286	HIS
1	D	297	GLU
1	D	300	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	11	GLN
1	A	48	ASN
1	A	54	GLN

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Mol	Chain	Res	Type
1	A	87	GLN
1	A	94	HIS
1	A	149	HIS
1	A	244	GLN
1	A	272	ASN
1	B	10	GLN
1	B	11	GLN
1	B	48	ASN
1	B	54	GLN
1	B	87	GLN
1	B	115	ASN
1	B	201	GLN
1	B	244	GLN
1	B	262	ASN
1	B	272	ASN
1	C	31	ASN
1	C	54	GLN
1	C	68	GLN
1	C	87	GLN
1	C	173	ASN
1	C	244	GLN
1	C	322	ASN
1	D	10	GLN
1	D	54	GLN
1	D	173	ASN
1	D	262	ASN
1	D	322	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 4 are unknown - leaving 6 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	C	343	-	46,48,48	1.88	14 (30%)	64,73,73	1.70	10 (15%)
2	NAD	D	343	-	46,48,48	1.80	10 (21%)	64,73,73	1.73	12 (18%)
4	SO4	A	345	-	4,4,4	0.43	0	6,6,6	0.41	0
4	SO4	A	346	-	4,4,4	0.16	0	6,6,6	0.70	0
2	NAD	B	343	-	46,48,48	1.77	9 (19%)	64,73,73	1.71	14 (21%)
2	NAD	A	343	-	46,48,48	1.64	10 (21%)	64,73,73	1.69	15 (23%)

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	C	343	-	-	5/30/62/62	0/5/5/5
2	NAD	B	343	-	-	6/30/62/62	0/5/5/5
2	NAD	A	343	-	-	6/30/62/62	0/5/5/5
2	NAD	D	343	-	-	5/30/62/62	0/5/5/5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	343	NAD	C2N-N1N	6.61	1.42	1.35
2	D	343	NAD	C2N-N1N	6.45	1.42	1.35
2	B	343	NAD	PN-O3	6.10	1.66	1.59
2	A	343	NAD	PN-O3	4.93	1.64	1.59
2	A	343	NAD	C2N-N1N	4.78	1.40	1.35
2	C	343	NAD	C6N-N1N	4.12	1.44	1.35
2	B	343	NAD	C2N-N1N	4.09	1.39	1.35
2	D	343	NAD	C6N-N1N	4.00	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	343	NAD	PA-O3	-3.44	1.55	1.59
2	B	343	NAD	C5A-N7A	-3.24	1.33	1.39
2	A	343	NAD	C4A-N9A	-3.01	1.31	1.37
2	B	343	NAD	C4A-N9A	-2.97	1.31	1.37
2	C	343	NAD	O4B-C1B	2.85	1.48	1.42
2	C	343	NAD	C7N-N7N	2.80	1.38	1.33
2	C	343	NAD	PN-O3	-2.75	1.56	1.59
2	D	343	NAD	PN-O2N	-2.75	1.42	1.55
2	D	343	NAD	C7N-N7N	2.74	1.38	1.33
2	A	343	NAD	C5A-N7A	-2.73	1.34	1.39
2	D	343	NAD	C5A-N7A	-2.72	1.34	1.39
2	B	343	NAD	PA-O3	2.70	1.62	1.59
2	D	343	NAD	PN-O3	-2.69	1.56	1.59
2	A	343	NAD	PA-O1A	-2.60	1.41	1.50
2	C	343	NAD	O4D-C1D	2.57	1.44	1.40
2	A	343	NAD	PN-O1N	-2.55	1.42	1.50
2	B	343	NAD	C6N-N1N	2.52	1.41	1.35
2	B	343	NAD	PA-O1A	-2.49	1.42	1.50
2	C	343	NAD	C4A-N9A	-2.38	1.32	1.37
2	C	343	NAD	PN-O2N	-2.34	1.44	1.55
2	C	343	NAD	C2N-C3N	2.27	1.42	1.39
2	B	343	NAD	C2A-N3A	-2.24	1.30	1.33
2	C	343	NAD	C5A-N7A	-2.22	1.35	1.39
2	C	343	NAD	O3D-C3D	2.21	1.48	1.43
2	D	343	NAD	PA-O2A	-2.20	1.45	1.55
2	B	343	NAD	C5D-C4D	2.20	1.58	1.51
2	C	343	NAD	PA-O2A	-2.11	1.45	1.55
2	A	343	NAD	O2D-C2D	-2.09	1.37	1.43
2	A	343	NAD	C6N-N1N	2.08	1.40	1.35
2	D	343	NAD	C5D-C4D	2.07	1.57	1.51
2	A	343	NAD	O4B-C4B	-2.04	1.40	1.45
2	C	343	NAD	C5B-C4B	2.03	1.57	1.51
2	D	343	NAD	C4A-N9A	-2.01	1.33	1.37
2	A	343	NAD	C3B-C4B	2.01	1.58	1.53
2	C	343	NAD	C8A-N9A	-2.01	1.34	1.37

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	343	NAD	N3A-C2A-N1A	-5.33	120.52	128.58
2	D	343	NAD	N3A-C2A-N1A	-5.14	120.80	128.58
2	C	343	NAD	C5A-C4A-N3A	-5.12	119.67	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	343	NAD	C5A-C4A-N3A	-4.85	120.04	126.72
2	D	343	NAD	C2N-C3N-C4N	4.74	123.78	118.26
2	B	343	NAD	C5A-C4A-N3A	-4.65	120.32	126.72
2	A	343	NAD	N3A-C2A-N1A	-4.36	121.98	128.58
2	C	343	NAD	C2A-N3A-C4A	4.27	122.25	111.83
2	B	343	NAD	C4A-C5A-N7A	-4.25	105.72	110.58
2	C	343	NAD	C2N-C3N-C4N	4.05	122.96	118.26
2	D	343	NAD	C2A-N3A-C4A	3.86	121.27	111.83
2	A	343	NAD	C5A-C4A-N3A	-3.80	121.49	126.72
2	B	343	NAD	C4D-O4D-C1D	-3.78	106.46	109.92
2	B	343	NAD	C5A-N7A-C8A	3.63	109.16	103.45
2	A	343	NAD	N9A-C8A-N7A	-3.60	108.83	113.94
2	B	343	NAD	N3A-C2A-N1A	-3.48	123.31	128.58
2	D	343	NAD	N9A-C8A-N7A	-3.42	109.08	113.94
2	D	343	NAD	N3A-C4A-N9A	3.40	132.95	127.17
2	A	343	NAD	C4A-N9A-C8A	3.40	109.31	105.74
2	A	343	NAD	C4A-C5A-N7A	-3.31	106.79	110.58
2	C	343	NAD	N9A-C8A-N7A	-3.18	109.42	113.94
2	A	343	NAD	C5A-N7A-C8A	3.13	108.38	103.45
2	C	343	NAD	N3A-C4A-N9A	3.12	132.47	127.17
2	A	343	NAD	O2A-PA-O3	-2.99	99.20	107.27
2	B	343	NAD	N9A-C8A-N7A	-2.98	109.70	113.94
2	A	343	NAD	C2A-N3A-C4A	2.94	119.01	111.83
2	A	343	NAD	C4D-O4D-C1D	-2.91	107.26	109.92
2	B	343	NAD	O2A-PA-O3	-2.87	99.51	107.27
2	C	343	NAD	C4A-C5A-N7A	-2.82	107.36	110.58
2	B	343	NAD	N3A-C4A-N9A	2.78	131.90	127.17
2	A	343	NAD	N3A-C4A-N9A	2.71	131.78	127.17
2	D	343	NAD	O7N-C7N-N7N	2.70	126.52	122.62
2	A	343	NAD	O2N-PN-O3	-2.68	100.02	107.27
2	B	343	NAD	C2A-N3A-C4A	2.64	118.28	111.83
2	D	343	NAD	C5A-N7A-C8A	2.64	107.60	103.45
2	A	343	NAD	C6N-N1N-C2N	-2.53	119.73	121.88
2	A	343	NAD	C2N-C3N-C4N	2.52	121.19	118.26
2	B	343	NAD	O2N-PN-O1N	2.45	123.86	112.44
2	C	343	NAD	C5A-N7A-C8A	2.43	107.27	103.45
2	D	343	NAD	C4A-N9A-C8A	2.40	108.26	105.74
2	A	343	NAD	O2N-PN-O1N	2.33	123.30	112.44
2	B	343	NAD	C2A-N1A-C6A	2.27	122.46	118.73
2	C	343	NAD	C4A-N9A-C8A	2.26	108.11	105.74
2	D	343	NAD	C4A-C5A-N7A	-2.25	108.01	110.58
2	A	343	NAD	C2A-N1A-C6A	2.22	122.38	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	343	NAD	C4D-O4D-C1D	2.22	111.95	109.92
2	B	343	NAD	O4D-C4D-C5D	-2.16	102.43	109.33
2	B	343	NAD	O2A-PA-O1A	2.09	122.17	112.44
2	C	343	NAD	C6N-N1N-C1D	-2.05	115.71	119.73
2	D	343	NAD	C4N-C3N-C7N	-2.02	115.55	121.06
2	B	343	NAD	C6N-N1N-C2N	-2.00	120.17	121.88

There are no chirality outliers.

All (22) torsion outliers are listed below:

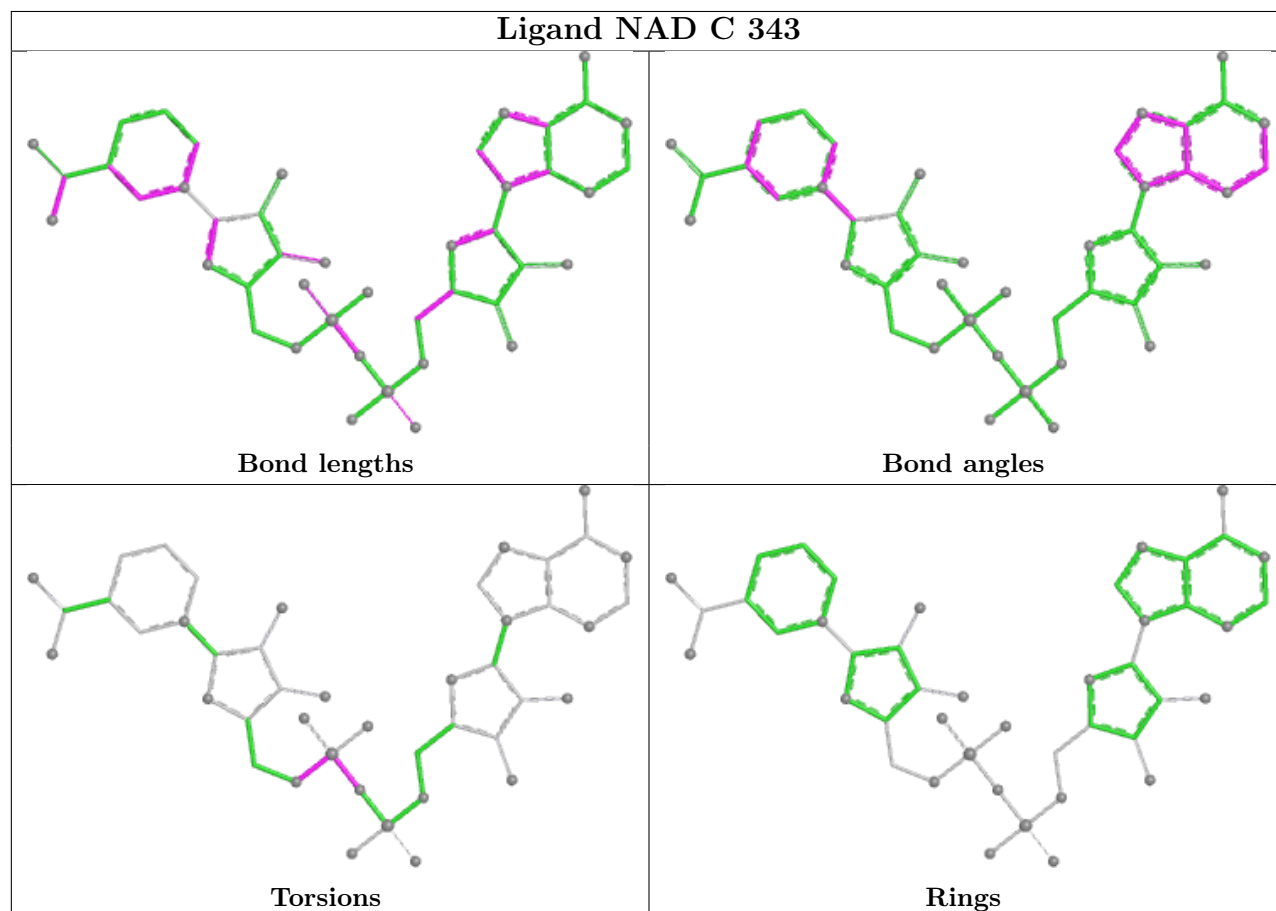
Mol	Chain	Res	Type	Atoms
2	A	343	NAD	C5B-O5B-PA-O2A
2	A	343	NAD	C5D-O5D-PN-O3
2	A	343	NAD	C5D-O5D-PN-O1N
2	B	343	NAD	C5B-O5B-PA-O2A
2	B	343	NAD	C5D-O5D-PN-O3
2	B	343	NAD	C5D-O5D-PN-O1N
2	C	343	NAD	C5D-O5D-PN-O3
2	C	343	NAD	C5D-O5D-PN-O1N
2	D	343	NAD	C5D-O5D-PN-O3
2	D	343	NAD	C5D-O5D-PN-O1N
2	A	343	NAD	PA-O3-PN-O1N
2	B	343	NAD	PA-O3-PN-O1N
2	C	343	NAD	PA-O3-PN-O1N
2	A	343	NAD	C5D-O5D-PN-O2N
2	B	343	NAD	C5D-O5D-PN-O2N
2	C	343	NAD	C5D-O5D-PN-O2N
2	D	343	NAD	C5D-O5D-PN-O2N
2	D	343	NAD	PA-O3-PN-O1N
2	A	343	NAD	PA-O3-PN-O2N
2	B	343	NAD	PA-O3-PN-O2N
2	C	343	NAD	PA-O3-PN-O2N
2	D	343	NAD	PA-O3-PN-O2N

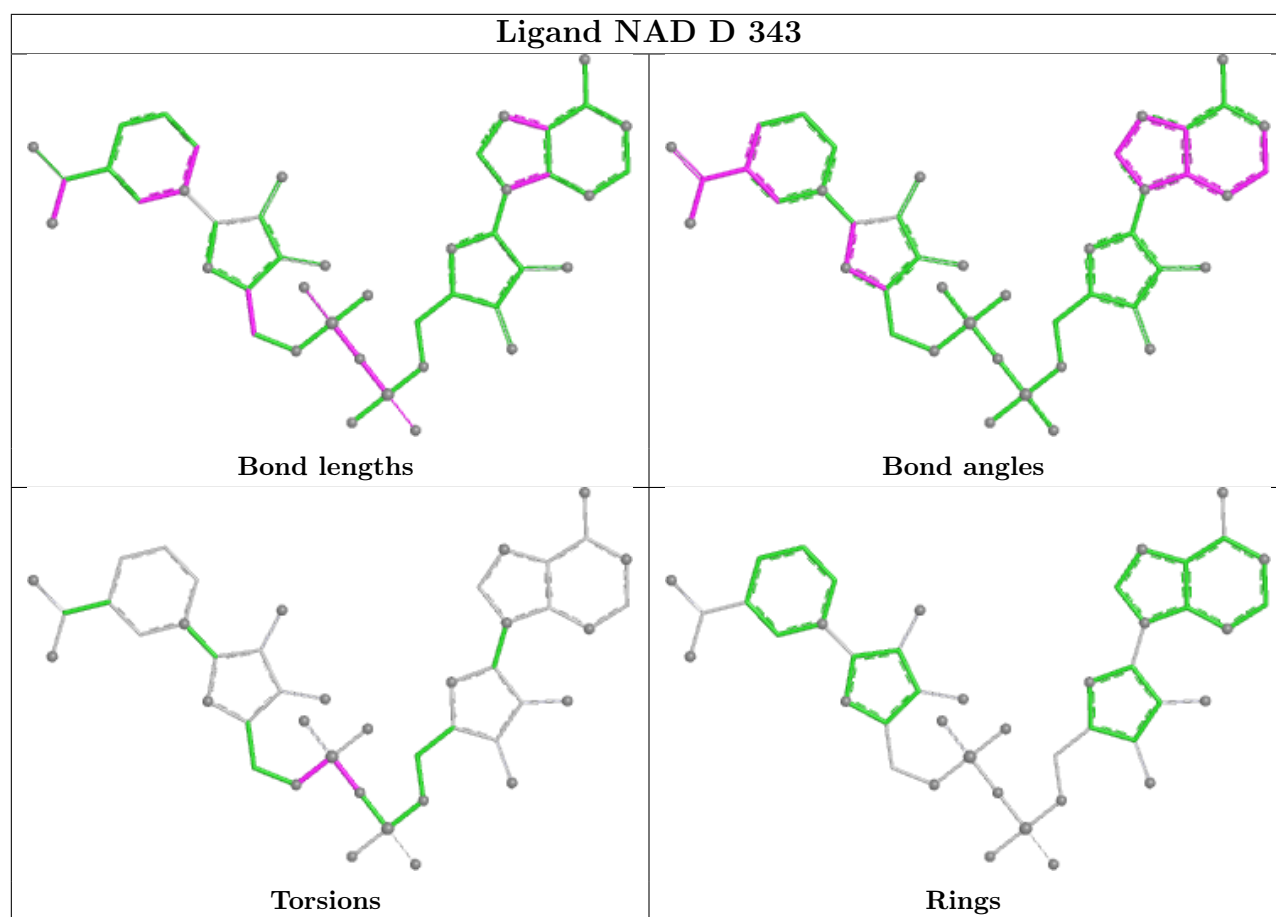
There are no ring outliers.

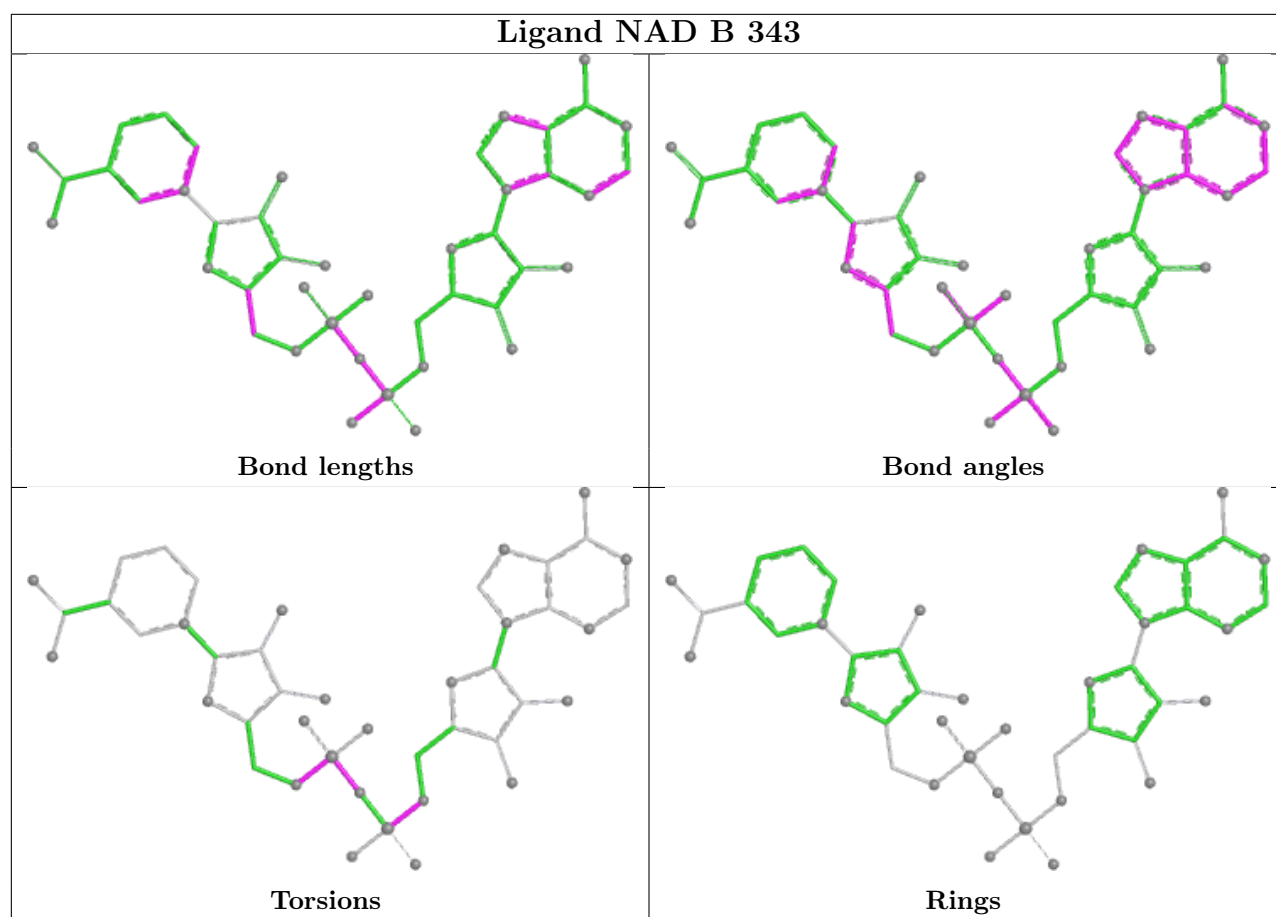
No monomer is involved in short contacts.

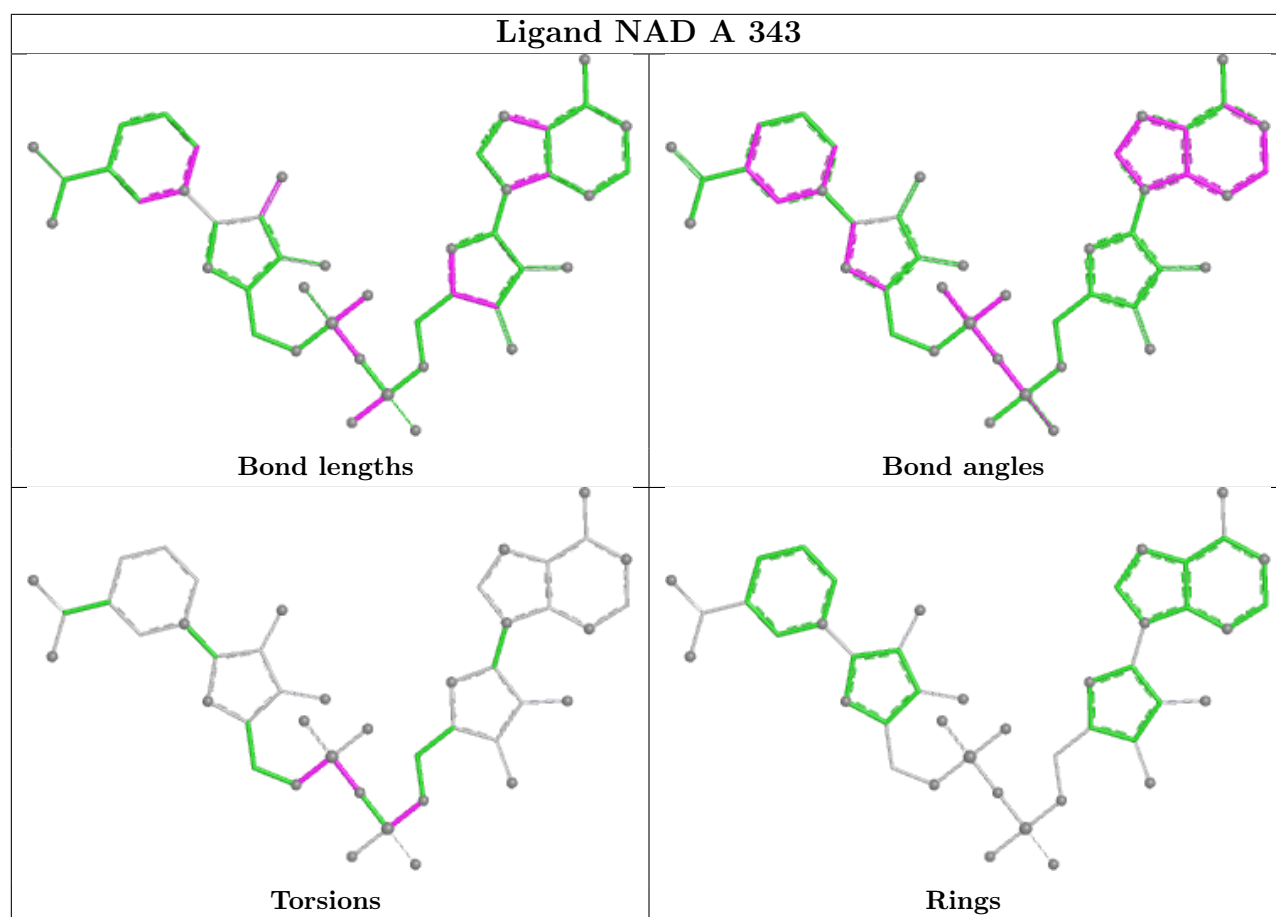
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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%)	0.25	26 (7%)	19 21	38, 62, 100, 124	0
1	B	336/351 (95%)	0.11	18 (5%)	31 33	38, 60, 95, 117	0
1	C	336/351 (95%)	-0.72	0	100 100	33, 43, 68, 96	0
1	D	336/351 (95%)	-1.11	0	100 100	22, 28, 42, 63	0
All	All	1344/1404 (95%)	-0.37	44 (3%)	49 51	22, 47, 91, 124	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	THR	3.4
1	B	132	ALA	3.1
1	B	226	ILE	3.0
1	A	14	PHE	2.9
1	B	128	ALA	2.8
1	A	84	THR	2.8
1	A	65	SER	2.8
1	A	132	ALA	2.8
1	A	129	ALA	2.7
1	B	131	ASN	2.7
1	A	111	PRO	2.7
1	A	68	GLN	2.6
1	B	84	THR	2.6
1	A	88	VAL	2.5
1	A	40	ASN	2.5
1	B	88	VAL	2.5
1	A	184	TYR	2.5
1	A	180	TYR	2.5
1	A	168	VAL	2.4
1	A	185	GLY	2.4
1	B	91	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	81	ASP	2.4
1	A	293	ILE	2.4
1	B	81	ASP	2.4
1	B	279	TYR	2.4
1	A	131	ASN	2.4
1	B	230	GLY	2.4
1	A	279	TYR	2.3
1	A	128	ALA	2.3
1	B	285	ILE	2.3
1	B	293	ILE	2.3
1	A	224	VAL	2.2
1	A	86	GLU	2.2
1	A	287	HIS	2.2
1	B	111	PRO	2.1
1	B	225	TYR	2.1
1	A	90	LYS	2.1
1	A	15	SER	2.1
1	A	124	ASN	2.1
1	B	277	TYR	2.1
1	A	298	PHE	2.1
1	B	305	HIS	2.1
1	B	127	HIS	2.0
1	B	183	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

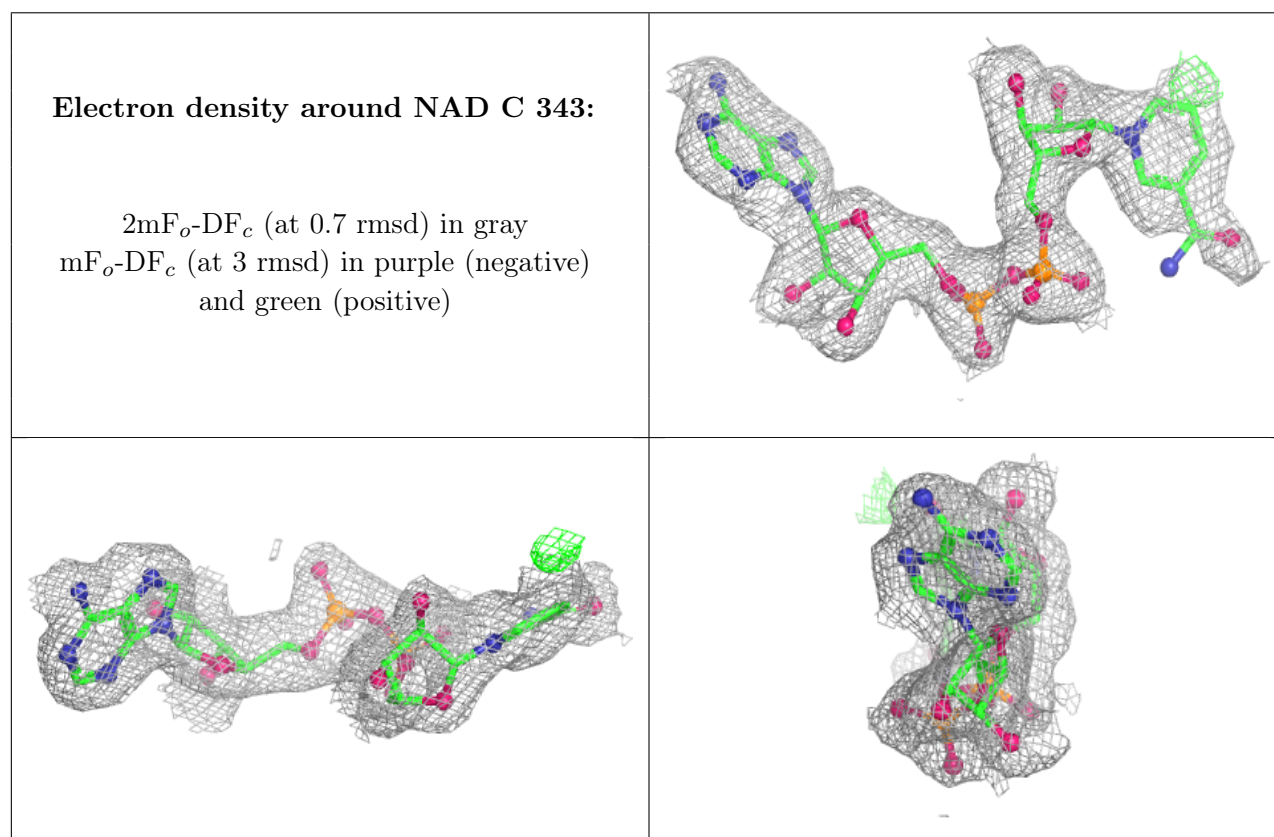
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

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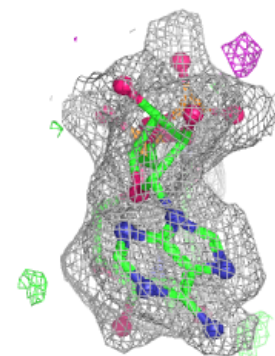
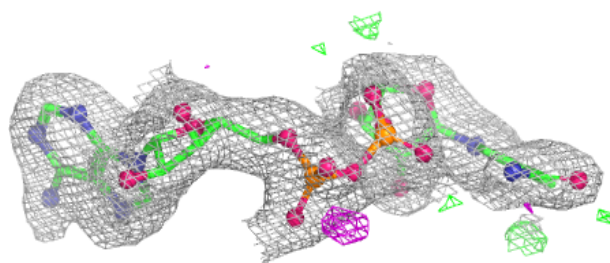
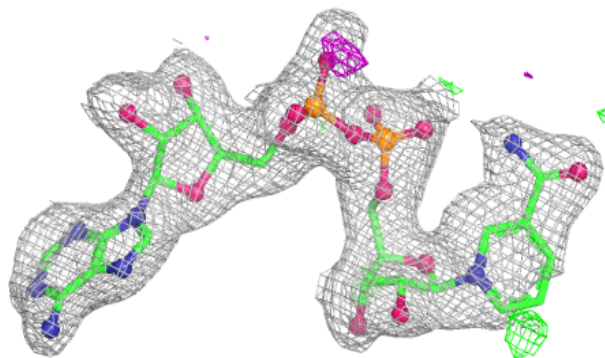
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UNL	B	344	25/-	0.97	0.07	46,65,72,76	0
3	UNL	A	344	25/-	0.98	0.06	45,65,71,76	0
2	NAD	C	343	44/44	0.99	0.04	24,30,44,46	0
2	NAD	D	343	44/44	0.99	0.03	20,28,41,45	0
2	NAD	A	343	44/44	0.99	0.03	25,30,42,46	0
2	NAD	B	343	44/44	0.99	0.04	24,30,42,45	0
3	UNL	C	344	25/-	0.99	0.04	39,44,48,50	0
3	UNL	D	344	25/-	0.99	0.03	26,33,37,38	0
4	SO4	A	345	5/5	1.00	0.02	28,29,31,33	0
4	SO4	A	346	5/5	1.00	0.02	30,30,33,34	0

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

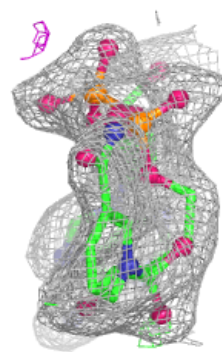
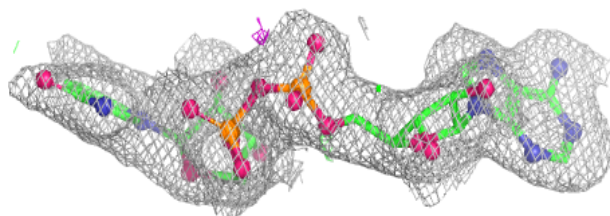
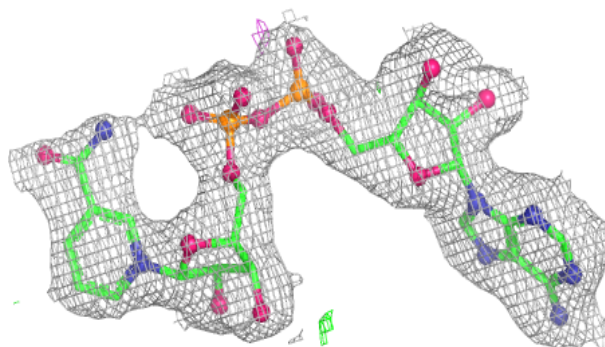


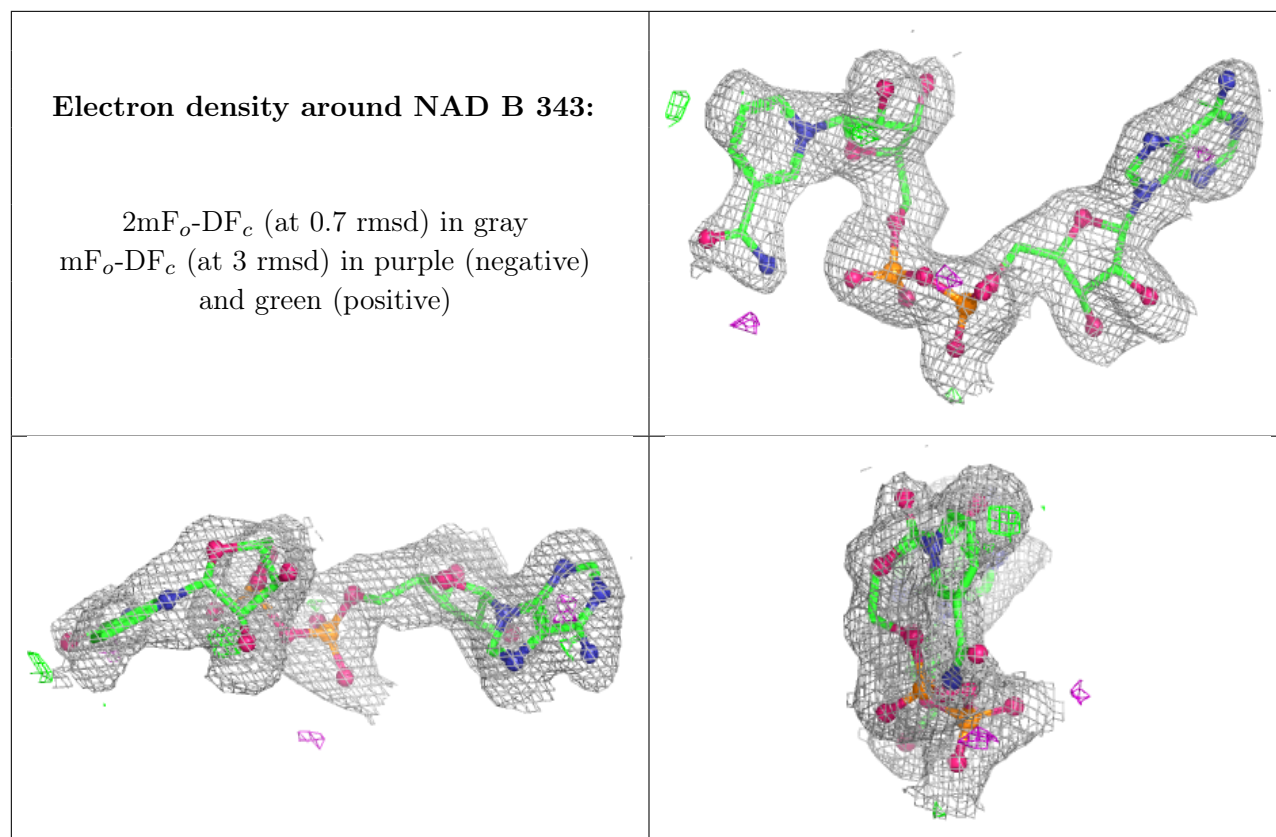
Electron density around NAD D 343:

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

**Electron density around NAD 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.