W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 17, 2024 – 07:20 AM EST

PDB ID	:	3RUF
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	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) 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	:	2.36
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)	:	2.36

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 2.00 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	Percentile Ranks	Value
Rfree		0.247
Ramachandran outliers		0.5%
Sidechain outliers		4.0%
RSRZ outliers		1.8%

Worse — *Better*

▉ Percentile relative to all X-ray structures
▊ Percentile relative to X-ray structures of similar resolution
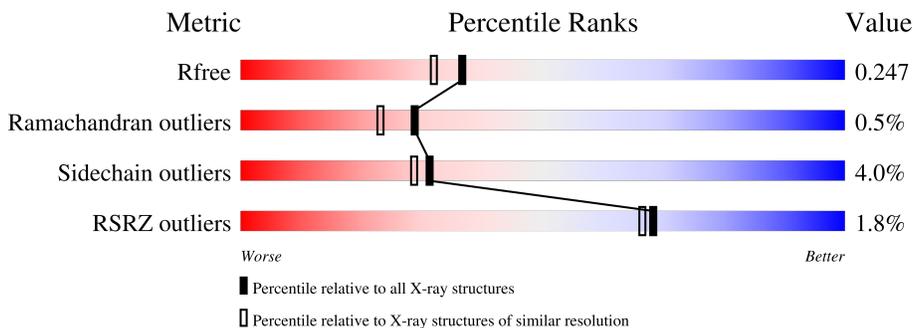
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	.% / 89% 6% · ·
1	B	351	2% / 89% 6% · ·
1	S	351	3% / 92% · ·
1	b	351	.% / 90% 5% ·

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 11427 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	S	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
			2674	1706	459	501	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
S	-8	HIS	-	expression tag	UNP Q7BJX9
S	-7	HIS	-	expression tag	UNP Q7BJX9
S	-6	HIS	-	expression tag	UNP Q7BJX9
S	-5	HIS	-	expression tag	UNP Q7BJX9
S	-4	HIS	-	expression tag	UNP Q7BJX9
S	-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

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| Chain	Residue	Modelled	Actual	Comment	Reference
b	-5	HIS	-	expression tag	UNP Q7BJX9
b	-4	HIS	-	expression tag	UNP Q7BJX9
b	-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	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	S	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		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).

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	S	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		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
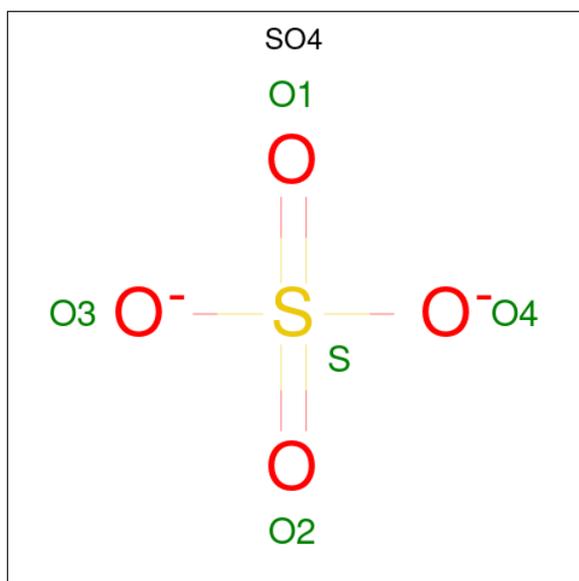
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total 111	O 111	0	0
5	B	115	Total 115	O 115	0	0
5	S	101	Total 101	O 101	0	0
5	b	102	Total 102	O 102	0	0

3　Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: WbgU

- Molecule 1: WbgU

- Molecule 1: WbgU

- Molecule 1: WbgU

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	77.98Å 77.98Å 223.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.00 – 2.00 37.32 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.1 (37.00-2.00) 58.4 (37.32-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.204 , 0.248 0.206 , 0.247	Depositor DCC
R_{free} test set	7537 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 32.6	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l 0.437 for h,-h-k,-l 0.027 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11427	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAD, UDP

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	1.10	9/2739 (0.3%)	0.92	2/3717 (0.1%)
1	B	1.17	11/2739 (0.4%)	0.96	8/3717 (0.2%)
1	S	1.03	0/2739	0.91	5/3717 (0.1%)
1	b	1.05	3/2731 (0.1%)	0.92	7/3706 (0.2%)
All	All	1.09	23/10948 (0.2%)	0.93	22/14857 (0.1%)

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	318	LYS	CD-CE	12.09	1.81	1.51
1	A	7	GLU	CB-CG	8.94	1.69	1.52
1	B	7	GLU	CB-CG	8.07	1.67	1.52
1	B	318	LYS	CB-CG	7.54	1.72	1.52
1	B	318	LYS	CE-NZ	7.39	1.67	1.49

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	258	ASP	CB-CG-OD2	7.34	124.91	118.30
1	B	299	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	239	ILE	CB-CA-C	-6.57	98.45	111.60
1	S	240	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	260	ILE	CG1-CB-CG2	-6.29	97.57	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	321 (97%)	10 (3%)	1 (0%)	41	37
1	B	332/351 (95%)	323 (97%)	7 (2%)	2 (1%)	25	19
1	S	332/351 (95%)	321 (97%)	9 (3%)	2 (1%)	25	19
1	b	332/351 (95%)	322 (97%)	8 (2%)	2 (1%)	25	19
All	All	1328/1404 (95%)	1287 (97%)	34 (3%)	7 (0%)	29	23

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	286	HIS
1	S	3	SER
1	B	286	HIS
1	b	103	SER
1	A	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	290/304 (95%)	275 (95%)	15 (5%)	23	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	290/304 (95%)	276 (95%)	14 (5%)	25	22
1	S	290/304 (95%)	283 (98%)	7 (2%)	49	51
1	b	289/304 (95%)	279 (96%)	10 (4%)	36	35
All	All	1159/1216 (95%)	1113 (96%)	46 (4%)	31	29

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	338	ARG
1	S	338	ARG
1	S	71	ARG
1	S	183	THR
1	b	15	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	283	ASN
1	b	195	ASN
1	b	173	ASN
1	B	149	HIS
1	S	195	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	#$|Z| > 2$
2	NAD	A	343	-	42,48,48	1.18	3 (7%)	50,73,73	1.85	11 (22%)
3	UDP	A	344	-	24,26,26	1.19	2 (8%)	37,40,40	1.83	11 (29%)
3	UDP	B	344	-	24,26,26	1.16	1 (4%)	37,40,40	1.73	8 (21%)
4	SO4	A	345	-	4,4,4	1.45	0	6,6,6	0.62	0
3	UDP	b	343	-	24,26,26	0.96	1 (4%)	37,40,40	1.55	8 (21%)
2	NAD	b	344	-	42,48,48	1.21	4 (9%)	50,73,73	1.64	11 (22%)
2	NAD	B	343	-	42,48,48	1.08	3 (7%)	50,73,73	1.80	10 (20%)
2	NAD	S	343	-	42,48,48	1.07	1 (2%)	50,73,73	1.63	7 (14%)
3	UDP	S	344	-	24,26,26	1.13	3 (12%)	37,40,40	1.51	8 (21%)

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	A	343	-	-	6/26/62/62	0/5/5/5
3	UDP	A	344	-	-	1/16/32/32	0/2/2/2
3	UDP	B	344	-	-	2/16/32/32	0/2/2/2
3	UDP	b	343	-	-	1/16/32/32	0/2/2/2
2	NAD	b	344	-	-	6/26/62/62	0/5/5/5
2	NAD	B	343	-	-	6/26/62/62	0/5/5/5
2	NAD	S	343	-	-	6/26/62/62	0/5/5/5
3	UDP	S	344	-	-	1/16/32/32	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	343	NAD	O4B-C1B	4.27	1.47	1.41
3	A	344	UDP	C2-N1	3.79	1.44	1.38
2	b	344	NAD	C7N-N7N	3.08	1.38	1.33
3	B	344	UDP	C2-N1	3.06	1.43	1.38
2	S	343	NAD	C7N-N7N	2.84	1.38	1.33

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	343	NAD	N3A-C2A-N1A	-7.05	117.67	128.68
2	S	343	NAD	N3A-C2A-N1A	-6.48	118.55	128.68
2	B	343	NAD	N3A-C2A-N1A	-6.11	119.13	128.68
2	b	344	NAD	N3A-C2A-N1A	-5.02	120.83	128.68
2	A	343	NAD	O7N-C7N-C3N	-4.90	113.77	119.63

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
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	S	343	NAD	C5D-O5D-PN-O1N
2	b	344	NAD	C5D-O5D-PN-O1N

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 then 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 NAD A 343

Bond lengths

Bond angles

Torsions

Rings

Ligand UDP A 344

Bond lengths

Bond angles

Torsions

Rings

Ligand UDP B 344

Bond lengths

Bond angles

Torsions

Rings

Ligand UDP b 343

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD b 344

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD B 343

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD S 343

Bond lengths

Bond angles

Torsions

Rings

Ligand UDP S 344


Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	336/351 (95%)	-0.27	4 (1%)	79	78	27, 38, 66, 82	0
1	B	336/351 (95%)	-0.25	6 (1%)	68	66	28, 39, 68, 83	0
1	S	336/351 (95%)	-0.15	9 (2%)	54	53	29, 41, 67, 92	0
1	b	336/351 (95%)	-0.12	5 (1%)	73	72	28, 41, 66, 85	0
All	All	1344/1404 (95%)	-0.20	24 (1%)	68	66	27, 40, 67, 92	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	b	2	MET	8.9
1	S	2	MET	6.0
1	B	286	HIS	4.9
1	B	301	GLY	4.6
1	b	1	TYR	4.6

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 monosaccharides 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, 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	UDP	A	344	25/25	0.91	0.12	47,50,53,54	0
3	UDP	b	343	25/25	0.92	0.09	38,49,52,52	0
2	NAD	b	344	44/44	0.94	0.10	30,36,41,45	0
2	NAD	A	343	44/44	0.95	0.10	23,31,38,41	0
2	NAD	B	343	44/44	0.95	0.10	27,32,39,40	0
3	UDP	B	344	25/25	0.95	0.09	45,51,53,54	0
3	UDP	S	344	25/25	0.95	0.09	42,48,49,52	0
2	NAD	S	343	44/44	0.95	0.11	29,35,40,44	0
4	SO4	A	345	5/5	0.99	0.11	30,30,30,30	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 UDP A 344:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
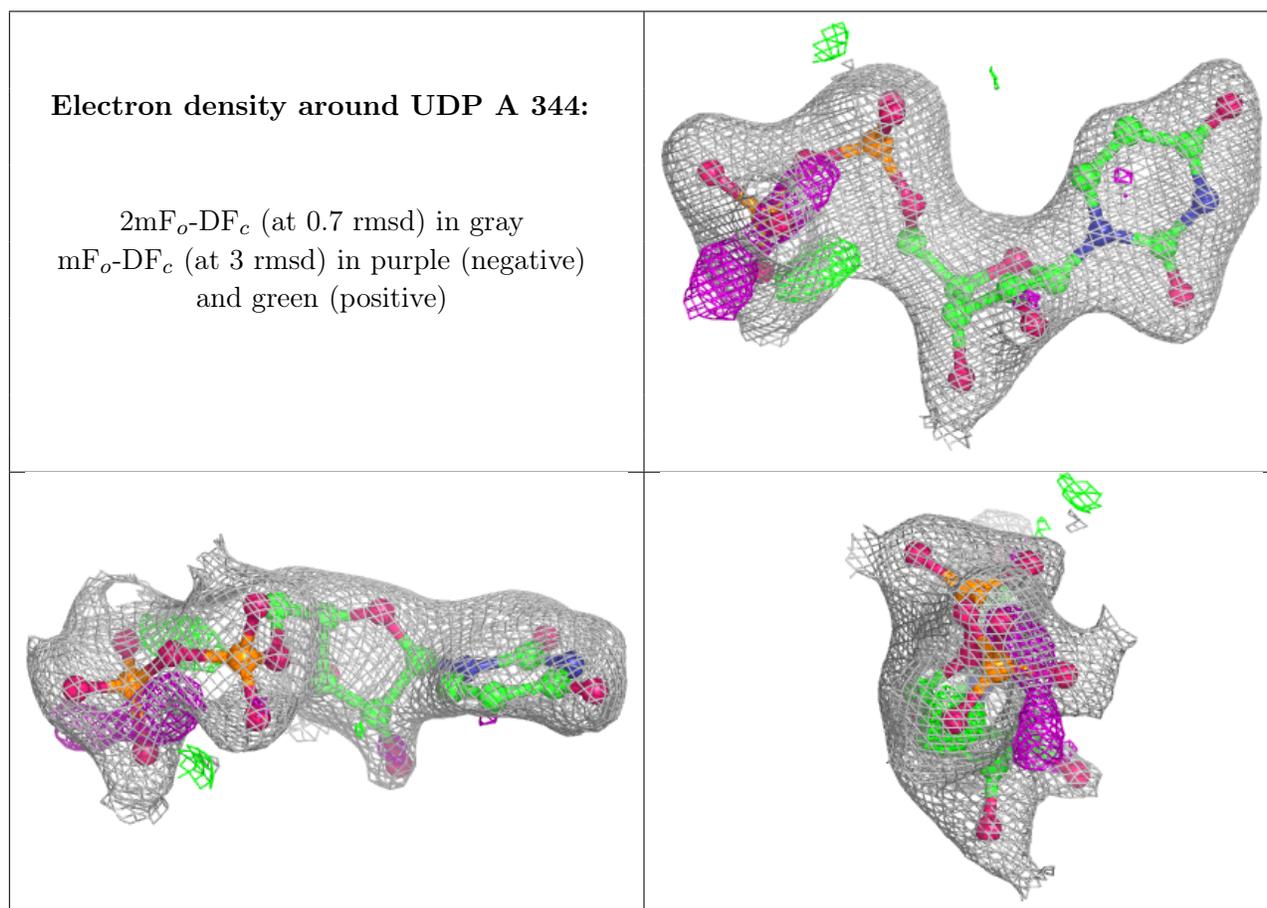
Electron density around UDP b 343:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
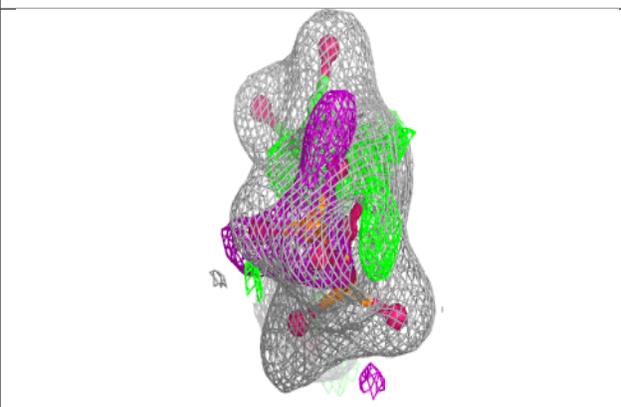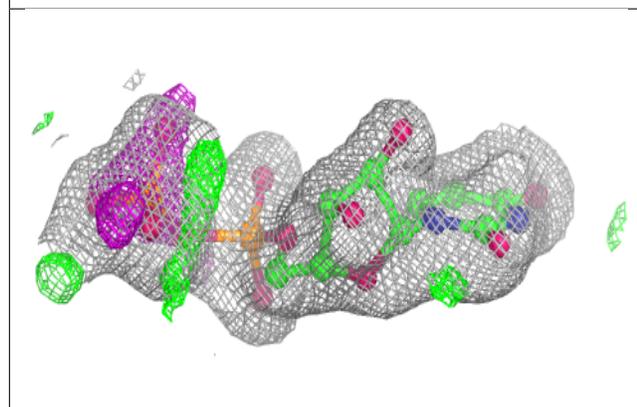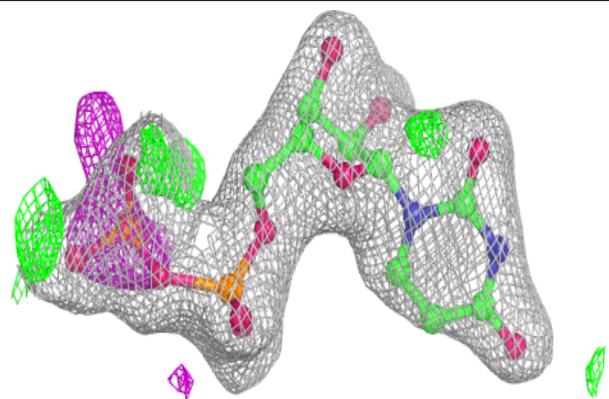
Electron density around NAD b 344:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
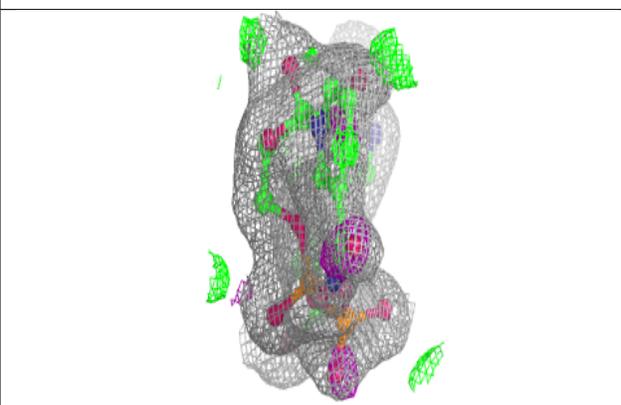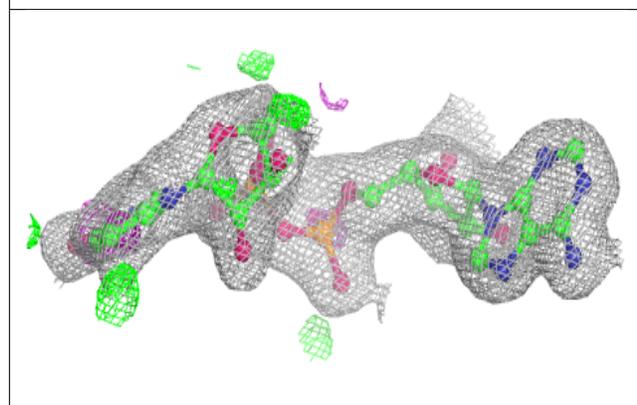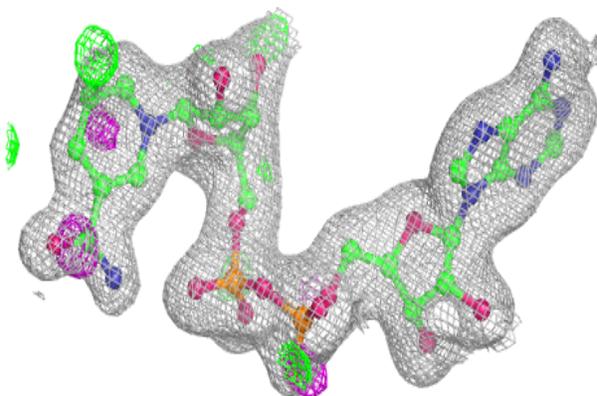
Electron density around NAD A 343:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
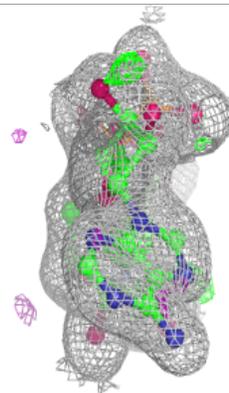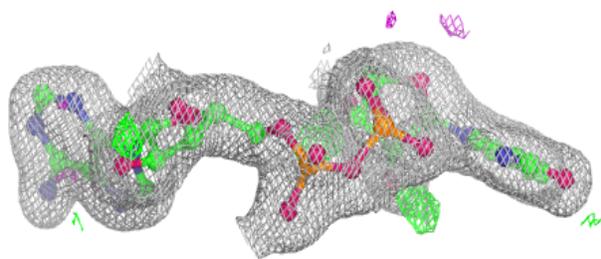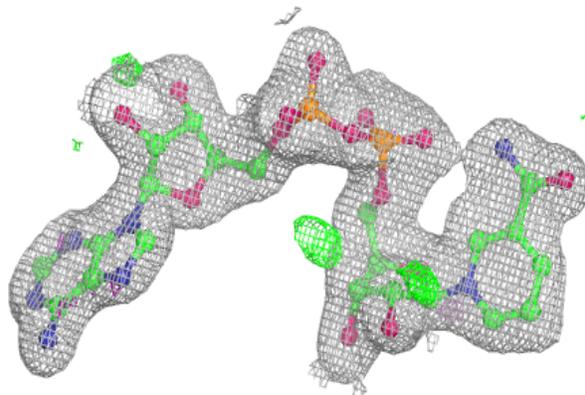
Electron density around NAD B 343:

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

Electron density around UDP 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 UDP S 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 S 343:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
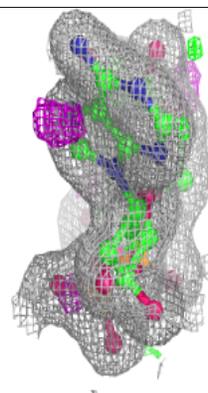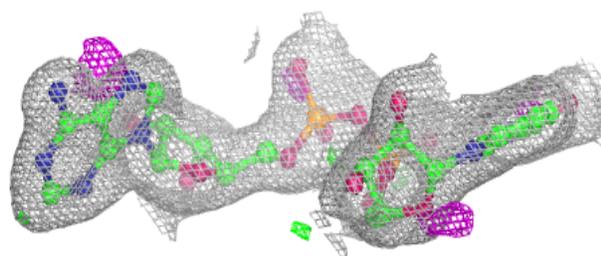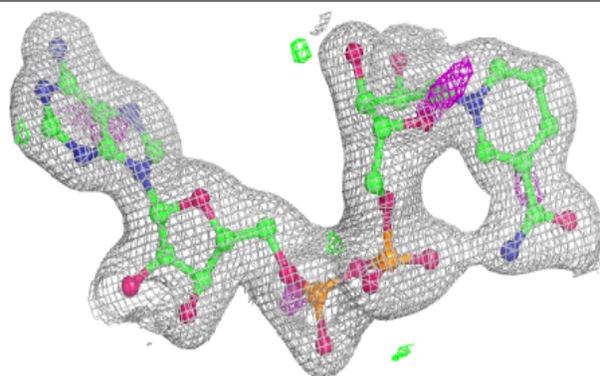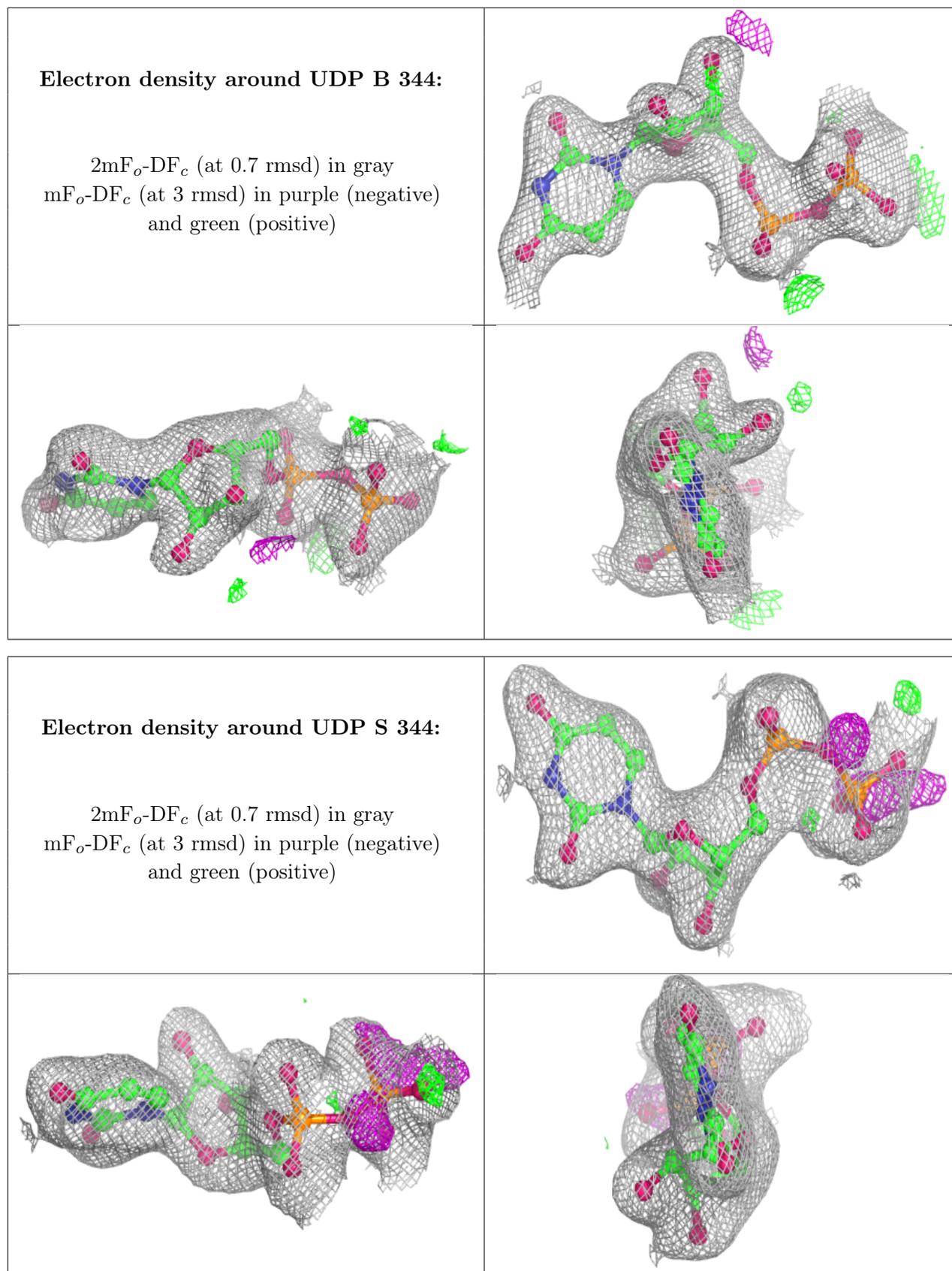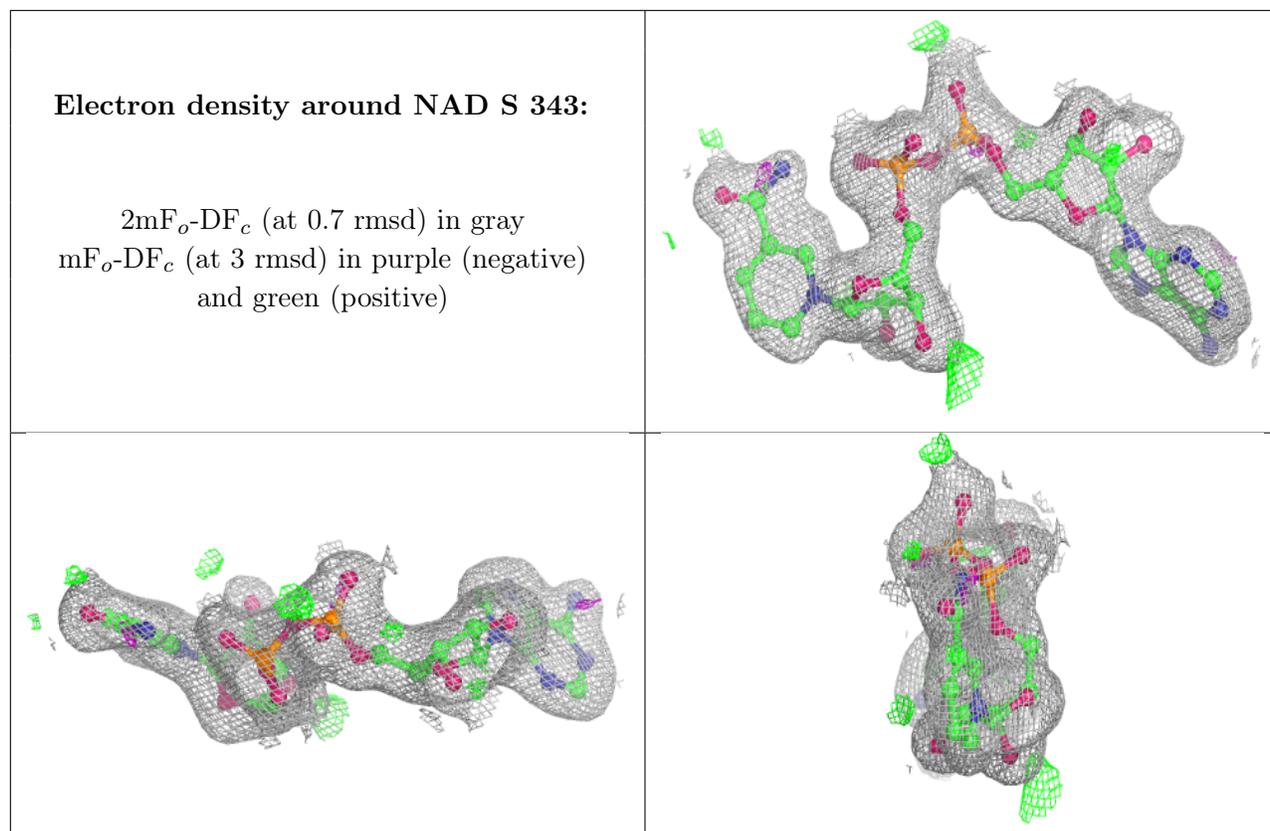
6.5 Other polymers (i)

There are no such residues in this entry.