WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2023 – 04:24 pm BST

PDB ID	:	8P2J
Title	:	Imine Reductase from Ajellomyces dermatitidis in space group C21
Authors	:	Sharma, M.; Grogan, G.
Deposited on	:	2023-05-16
Resolution	:	1.73 Å(reported)

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

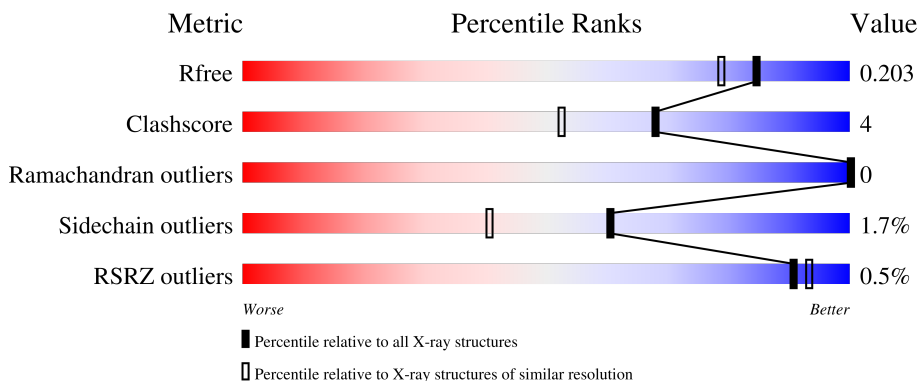|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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.
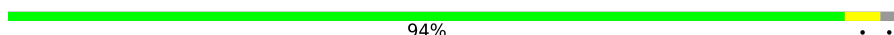
Metric	Percentile Ranks	Value
Rfree		0.203
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		1.7%
RSRZ outliers		0.5%

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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	294	91% 6% ·
1	B	294	89% 8% ··
1	C	294	% 93% 6%
1	D	294	87% 10% ··
1	E	294	2% 88% 11% ·

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Mol	Chain	Length	Quality of chain
1	F	294	90% ⠀⠀⠀7% ·
1	G	294	% ⠀⠀91% ⠀⠀9%
1	H	294	85% ⠀⠀9% · ·
1	I	294	94% ⠀⠀· ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 21304 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 Oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	1	0
			2088	1333	352	392	11			
1	B	288	Total	C	N	O	S	0	0	0
			2080	1328	354	386	12			
1	C	293	Total	C	N	O	S	0	1	0
			2136	1362	361	400	13			
1	D	288	Total	C	N	O	S	0	2	0
			2094	1339	353	390	12			
1	E	293	Total	C	N	O	S	0	1	0
			2127	1357	361	398	11			
1	F	288	Total	C	N	O	S	0	1	0
			2098	1337	353	396	12			
1	G	293	Total	C	N	O	S	0	1	0
			2135	1361	361	401	12			
1	H	281	Total	C	N	O	S	0	2	0
			2062	1317	348	387	10			
1	I	288	Total	C	N	O	S	0	0	0
			2099	1336	356	395	12			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP A0A179UH34
A	-4	PHE	-	expression tag	UNP A0A179UH34
A	-3	GLN	-	expression tag	UNP A0A179UH34
A	-2	GLY	-	expression tag	UNP A0A179UH34
A	-1	PRO	-	expression tag	UNP A0A179UH34
A	0	ALA	-	expression tag	UNP A0A179UH34
A	140	GLU	ALA	engineered mutation	UNP A0A179UH34
B	-5	LEU	-	expression tag	UNP A0A179UH34
B	-4	PHE	-	expression tag	UNP A0A179UH34
B	-3	GLN	-	expression tag	UNP A0A179UH34
B	-2	GLY	-	expression tag	UNP A0A179UH34

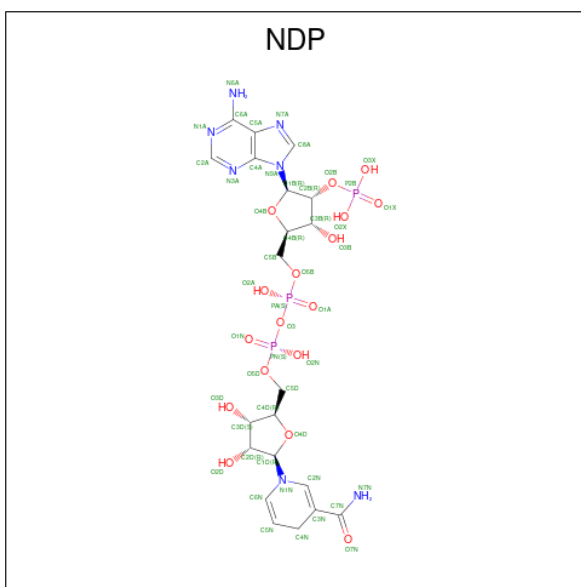*Continued on next page...*

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	PRO	-	expression tag	UNP A0A179UH34
B	0	ALA	-	expression tag	UNP A0A179UH34
B	140	GLU	ALA	engineered mutation	UNP A0A179UH34
C	-5	LEU	-	expression tag	UNP A0A179UH34
C	-4	PHE	-	expression tag	UNP A0A179UH34
C	-3	GLN	-	expression tag	UNP A0A179UH34
C	-2	GLY	-	expression tag	UNP A0A179UH34
C	-1	PRO	-	expression tag	UNP A0A179UH34
C	0	ALA	-	expression tag	UNP A0A179UH34
C	140	GLU	ALA	engineered mutation	UNP A0A179UH34
D	-5	LEU	-	expression tag	UNP A0A179UH34
D	-4	PHE	-	expression tag	UNP A0A179UH34
D	-3	GLN	-	expression tag	UNP A0A179UH34
D	-2	GLY	-	expression tag	UNP A0A179UH34
D	-1	PRO	-	expression tag	UNP A0A179UH34
D	0	ALA	-	expression tag	UNP A0A179UH34
D	140	GLU	ALA	engineered mutation	UNP A0A179UH34
E	-5	LEU	-	expression tag	UNP A0A179UH34
E	-4	PHE	-	expression tag	UNP A0A179UH34
E	-3	GLN	-	expression tag	UNP A0A179UH34
E	-2	GLY	-	expression tag	UNP A0A179UH34
E	-1	PRO	-	expression tag	UNP A0A179UH34
E	0	ALA	-	expression tag	UNP A0A179UH34
E	140	GLU	ALA	engineered mutation	UNP A0A179UH34
F	-5	LEU	-	expression tag	UNP A0A179UH34
F	-4	PHE	-	expression tag	UNP A0A179UH34
F	-3	GLN	-	expression tag	UNP A0A179UH34
F	-2	GLY	-	expression tag	UNP A0A179UH34
F	-1	PRO	-	expression tag	UNP A0A179UH34
F	0	ALA	-	expression tag	UNP A0A179UH34
F	140	GLU	ALA	engineered mutation	UNP A0A179UH34
G	-5	LEU	-	expression tag	UNP A0A179UH34
G	-4	PHE	-	expression tag	UNP A0A179UH34
G	-3	GLN	-	expression tag	UNP A0A179UH34
G	-2	GLY	-	expression tag	UNP A0A179UH34
G	-1	PRO	-	expression tag	UNP A0A179UH34
G	0	ALA	-	expression tag	UNP A0A179UH34
G	140	GLU	ALA	engineered mutation	UNP A0A179UH34
H	-5	LEU	-	expression tag	UNP A0A179UH34
H	-4	PHE	-	expression tag	UNP A0A179UH34
H	-3	GLN	-	expression tag	UNP A0A179UH34
H	-2	GLY	-	expression tag	UNP A0A179UH34

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	PRO	-	expression tag	UNP A0A179UH34
H	0	ALA	-	expression tag	UNP A0A179UH34
H	140	GLU	ALA	engineered mutation	UNP A0A179UH34
I	-5	LEU	-	expression tag	UNP A0A179UH34
I	-4	PHE	-	expression tag	UNP A0A179UH34
I	-3	GLN	-	expression tag	UNP A0A179UH34
I	-2	GLY	-	expression tag	UNP A0A179UH34
I	-1	PRO	-	expression tag	UNP A0A179UH34
I	0	ALA	-	expression tag	UNP A0A179UH34
I	140	GLU	ALA	engineered mutation	UNP A0A179UH34

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	234	Total	O	0	0
			234	234		
3	B	201	Total	O	0	0
			201	201		
3	C	264	Total	O	0	0
			264	264		
3	D	250	Total	O	0	0
			250	250		
3	E	204	Total	O	0	0
			204	204		
3	F	192	Total	O	0	0
			192	192		
3	G	189	Total	O	0	0
			189	189		
3	H	179	Total	O	0	0
			179	179		
3	I	240	Total	O	0	0
			240	240		

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: Oxidoreductase

Chain A:

- Molecule 1: Oxidoreductase

Chain B:

- Molecule 1: Oxidoreductase

Chain C:

- Molecule 1: Oxidoreductase
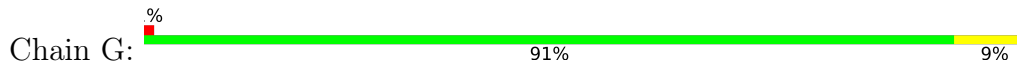
Chain D:

- Molecule 1: Oxidoreductase

Chain E:

A242 P243 Q260 L282 K288

• Molecule 1: Oxidoreductase

Chain F:

90%　　　　7%　·

LEU PHE GLN GLY ALA M1 Q21 K25 I64 V90 R101 Y114 I115 H116 G117 F124 L134 T148 V151 H168 Q204 A242 P243 N244 E247 I259 Q260 M287 K288

• Molecule 1: Oxidoreductase

Chain G:

%

91%　　　　9%

LEU F-4 P-1 A0 S4 Q21 R24 H27 I64 V90 R113 Y114 I115 H116 G117 F124 M125 L134 H168 H185 Q204 A242 P243 E247 Q250 Q260 K264 E272 M287 K288

• Molecule 1: Oxidoreductase

Chain H:

85%　　　　9%　·　·

LEU PHE GLN GLY PRO ALA MET ALA ASN S4 L11 Q21 F22 V31 W32 N33 I43 H49 L62 L63 I64 Q67 Q75 L92 Y114 I115 H116 G117 A121 F124 P129 L134 V151 T156 H168 H185 Q204 Y228 GLY ASP

GLY GLY S233 S234 L235 Q238 A242 P243 Q260 K288

• Molecule 1: Oxidoreductase

Chain I:

94%　　　　·　·

LEU PHE GLN GLY PRO ALA M1 Q21 H27 I64 V90 Y114 I115 H116 G117 L134 H168 E225 M237 L265 K288

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	204.62Å　87.97Å　162.58Å 90.00°　108.45°　90.00°	Depositor
Resolution (Å)	97.16　–　1.73 97.16　–　1.73	Depositor EDS
% Data completeness (in resolution range)	97.8 (97.16-1.73) 97.8 (97.16-1.73)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.166　,　0.193 0.178　,　0.203	Depositor DCC
R_{free} test set	13858 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.5	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21304	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.47% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NDP

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	0.48	0/2132	0.67	0/2905
1	B	0.45	0/2121	0.66	1/2892 (0.0%)
1	C	0.49	0/2182	0.69	0/2973
1	D	0.50	1/2141 (0.0%)	0.67	0/2917
1	E	0.45	0/2173	0.67	0/2962
1	F	0.45	0/2142	0.68	2/2919 (0.1%)
1	G	0.45	0/2181	0.67	0/2972
1	H	0.44	0/2108	0.67	0/2874
1	I	0.46	0/2140	0.68	0/2916
All	All	0.46	1/19320 (0.0%)	0.67	3/26330 (0.0%)

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
1	E	0	1
1	G	0	1
1	H	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	140	GLU	CD-OE1	5.19	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	101	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	F	101	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	128	GLN	CB-CG-CD	5.12	124.91	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	67	GLN	Mainchain
1	E	67	GLN	Mainchain
1	G	113	ARG	Sidechain
1	H	67	GLN	Mainchain

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	2088	0	2099	12	0
1	B	2080	0	2085	18	0
1	C	2136	0	2143	14	0
1	D	2094	0	2108	25	0
1	E	2127	0	2133	27	0
1	F	2098	0	2106	19	0
1	G	2135	0	2141	17	0
1	H	2062	0	2066	20	0
1	I	2099	0	2108	8	0
2	A	48	0	26	0	0
2	B	48	0	26	0	0
2	C	48	0	26	0	0
2	D	48	0	26	1	0
2	E	48	0	26	1	0
2	F	48	0	26	0	0
2	G	48	0	26	0	0
2	H	48	0	26	3	0
2	I	48	0	26	0	0
3	A	234	0	0	4	0
3	B	201	0	0	6	0
3	C	264	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	250	0	0	9	0
3	E	204	0	0	8	0
3	F	192	0	0	3	1
3	G	189	0	0	7	1
3	H	179	0	0	4	0
3	I	240	0	0	5	0
All	All	21304	0	19223	145	1

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 4.

The worst 5 of 145 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:E:260:GLN:HG3	3:E:548:HOH:O	1.61	0.98
1:G:125:MET:HG2	3:G:402:HOH:O	1.64	0.97
1:F:25:LYS:HG3	1:F:151:VAL:CG2	2.05	0.87
1:A:125:MET:HG2	3:A:401:HOH:O	1.77	0.83
1:F:25:LYS:HG3	1:F:151:VAL:HG21	1.67	0.77

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:587:HOH:O	3:G:554:HOH:O[3_445]	2.06	0.14

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	286/294 (97%)	282 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	286/294 (97%)	282 (99%)	4 (1%)	0	100	100
1	C	292/294 (99%)	287 (98%)	5 (2%)	0	100	100
1	D	288/294 (98%)	284 (99%)	4 (1%)	0	100	100
1	E	292/294 (99%)	288 (99%)	4 (1%)	0	100	100
1	F	287/294 (98%)	281 (98%)	6 (2%)	0	100	100
1	G	292/294 (99%)	285 (98%)	7 (2%)	0	100	100
1	H	279/294 (95%)	275 (99%)	4 (1%)	0	100	100
1	I	286/294 (97%)	282 (99%)	4 (1%)	0	100	100
All	All	2588/2646 (98%)	2546 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	210/221 (95%)	207 (99%)	3 (1%)	67	50
1	B	206/221 (93%)	202 (98%)	4 (2%)	57	36
1	C	215/221 (97%)	212 (99%)	3 (1%)	67	50
1	D	209/221 (95%)	203 (97%)	6 (3%)	42	18
1	E	213/221 (96%)	208 (98%)	5 (2%)	50	27
1	F	212/221 (96%)	210 (99%)	2 (1%)	78	67
1	G	215/221 (97%)	213 (99%)	2 (1%)	78	67
1	H	208/221 (94%)	200 (96%)	8 (4%)	33	11
1	I	212/221 (96%)	211 (100%)	1 (0%)	88	83
All	All	1900/1989 (96%)	1866 (98%)	34 (2%)	60	38

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	134	LEU
1	H	151	VAL
1	H	260	GLN
1	D	108	LEU
1	D	78[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	27	HIS
1	F	128	GLN
1	I	222	GLN
1	H	168	HIS
1	E	94	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	NDP	F	301	-	45,52,52	0.88	1 (2%)	53,80,80	0.95	2 (3%)
2	NDP	C	301	-	45,52,52	0.84	1 (2%)	53,80,80	0.87	1 (1%)
2	NDP	D	301	-	45,52,52	0.69	1 (2%)	53,80,80	1.01	3 (5%)
2	NDP	I	301	-	45,52,52	0.71	0	53,80,80	0.93	4 (7%)
2	NDP	A	301	-	45,52,52	0.74	1 (2%)	53,80,80	0.92	2 (3%)
2	NDP	B	301	-	45,52,52	0.67	0	53,80,80	0.99	5 (9%)
2	NDP	H	301	-	45,52,52	0.78	1 (2%)	53,80,80	0.95	3 (5%)
2	NDP	G	301	-	45,52,52	0.74	1 (2%)	53,80,80	0.88	1 (1%)
2	NDP	E	301	-	45,52,52	0.83	1 (2%)	53,80,80	0.86	1 (1%)

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	NDP	F	301	-	-	4/30/77/77	0/5/5/5
2	NDP	C	301	-	-	8/30/77/77	0/5/5/5
2	NDP	D	301	-	-	2/30/77/77	0/5/5/5
2	NDP	I	301	-	-	4/30/77/77	0/5/5/5
2	NDP	A	301	-	-	6/30/77/77	0/5/5/5
2	NDP	B	301	-	-	7/30/77/77	0/5/5/5
2	NDP	H	301	-	-	3/30/77/77	0/5/5/5
2	NDP	G	301	-	-	6/30/77/77	0/5/5/5
2	NDP	E	301	-	-	5/30/77/77	0/5/5/5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NDP	P2B-O2B	4.04	1.66	1.59
2	C	301	NDP	P2B-O2B	3.56	1.66	1.59
2	E	301	NDP	P2B-O2B	3.00	1.65	1.59
2	H	301	NDP	P2B-O2B	2.60	1.64	1.59
2	A	301	NDP	P2B-O2B	2.56	1.64	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	NDP	C5A-C6A-N6A	3.05	124.98	120.35
2	C	301	NDP	C3B-C2B-C1B	-2.94	97.37	102.89
2	A	301	NDP	C3B-C2B-C1B	-2.75	97.72	102.89
2	H	301	NDP	C3B-C2B-C1B	-2.73	97.75	102.89
2	D	301	NDP	C3B-C2B-C1B	-2.69	97.83	102.89

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	NDP	C2B-O2B-P2B-O2X
2	B	301	NDP	C5D-O5D-PN-O1N
2	C	301	NDP	C5D-O5D-PN-O1N
2	G	301	NDP	C5D-O5D-PN-O1N
2	A	301	NDP	C5D-O5D-PN-O3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	NDP	1	0
2	H	301	NDP	3	0
2	E	301	NDP	1	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 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 NDP F 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP I 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP A 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP H 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP G 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP E 301

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(Å^2)	Q<0.9
1	A	287/294 (97%)	-0.61	1 (0%)	94	95	17, 26, 44, 67	0
1	B	288/294 (97%)	-0.55	0	100	100	18, 26, 48, 82	0
1	C	293/294 (99%)	-0.62	3 (1%)	82	87	18, 24, 41, 69	0
1	D	288/294 (97%)	-0.61	0	100	100	17, 24, 43, 65	0
1	E	293/294 (99%)	-0.51	6 (2%)	65	71	19, 27, 53, 77	0
1	F	288/294 (97%)	-0.58	0	100	100	21, 30, 48, 69	0
1	G	293/294 (99%)	-0.54	3 (1%)	82	87	21, 28, 46, 76	0
1	H	281/294 (95%)	-0.61	0	100	100	20, 28, 47, 77	0
1	I	288/294 (97%)	-0.65	1 (0%)	94	95	18, 26, 45, 69	0
All	All	2599/2646 (98%)	-0.58	14 (0%)	91	93	17, 27, 47, 82	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	-4	PHE	6.0
1	A	2	ALA	5.6
1	G	-1	PRO	4.1
1	E	0	ALA	4.0
1	E	-3	GLN	3.8

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.

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wwPDB
PROTEIN DATA BANK

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
2	NDP	G	301	48/48	0.95	0.09	30,36,46,50	0
2	NDP	B	301	48/48	0.96	0.07	24,31,38,39	0
2	NDP	F	301	48/48	0.96	0.09	32,37,46,49	0
2	NDP	A	301	48/48	0.96	0.11	27,36,54,54	0
2	NDP	I	301	48/48	0.96	0.09	25,32,46,50	0
2	NDP	C	301	48/48	0.97	0.07	23,30,37,38	0
2	NDP	H	301	48/48	0.98	0.06	19,23,25,26	0
2	NDP	D	301	48/48	0.99	0.05	16,19,21,23	0
2	NDP	E	301	48/48	0.99	0.05	20,23,27,28	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.
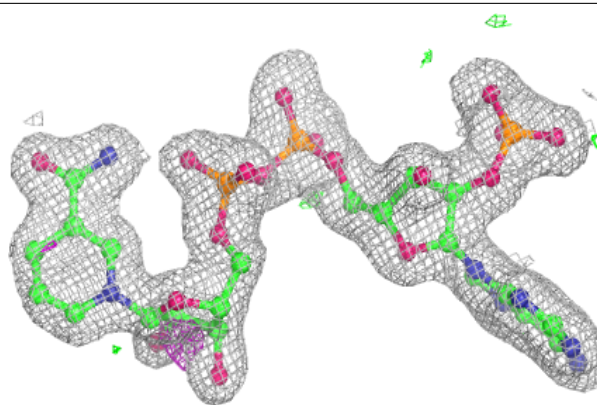
Electron density around NDP G 301:

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

Electron density around NDP B 301:

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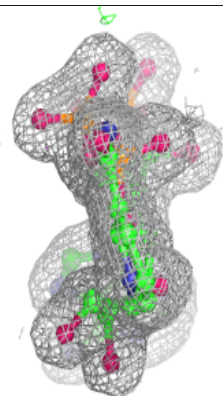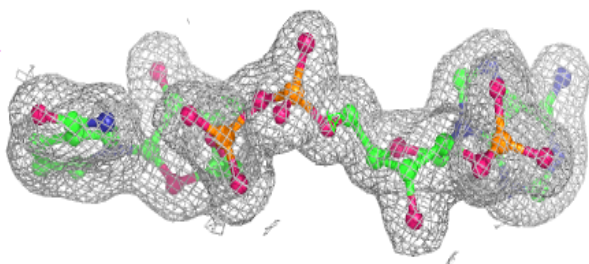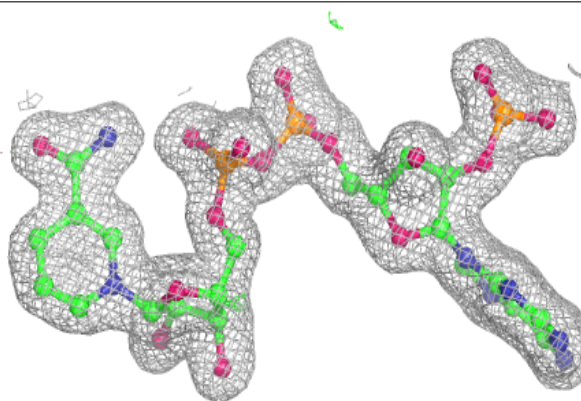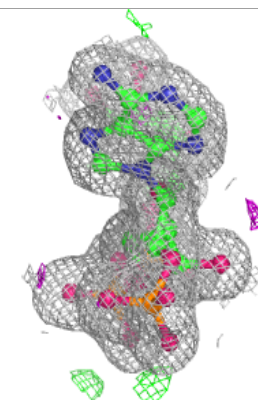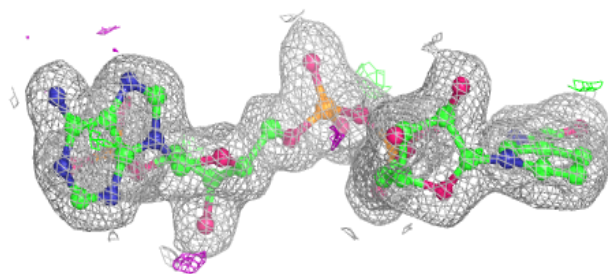mF_o-DF_c (at 3 rmsd) in purple (negative)
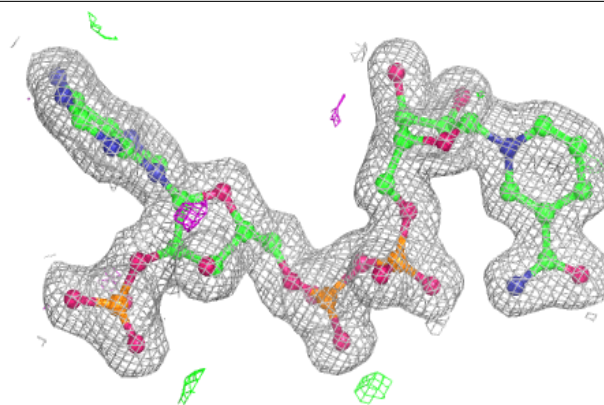and green (positive)


Electron density around NDP F 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
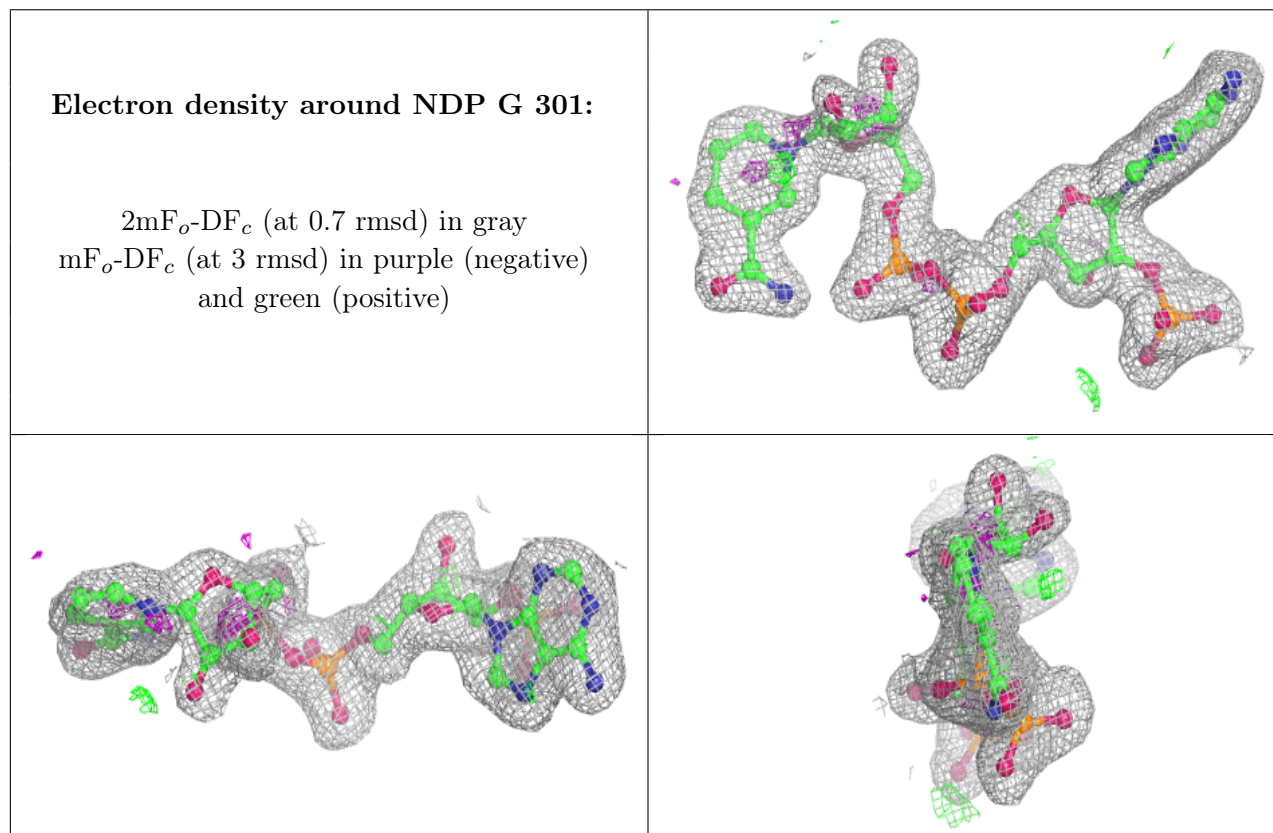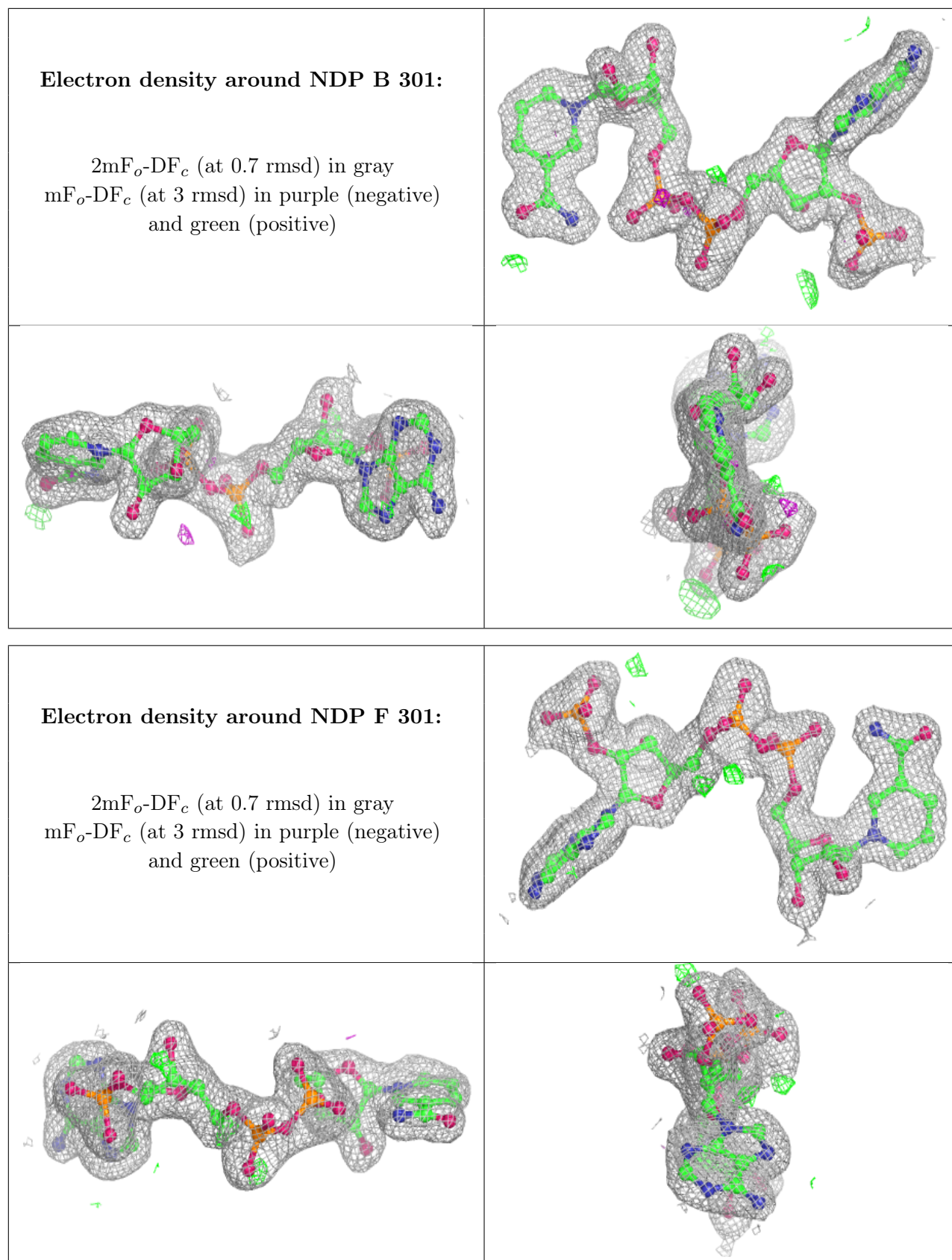
Electron density around NDP A 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
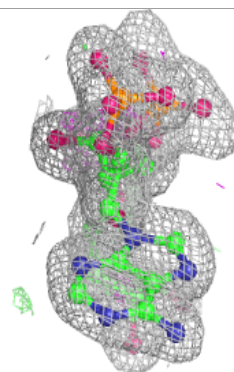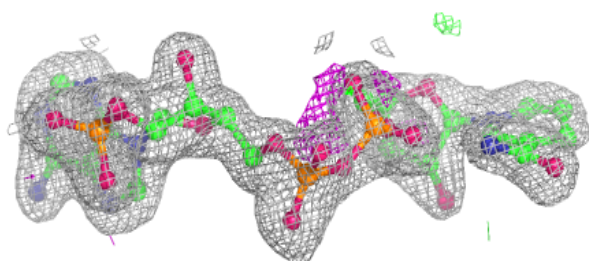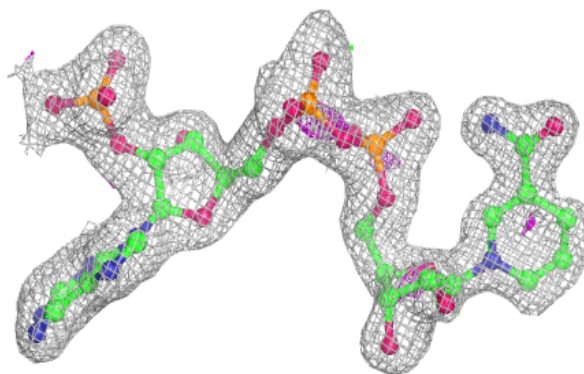
Electron density around NDP I 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
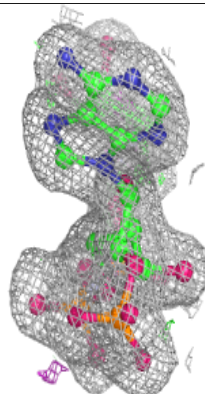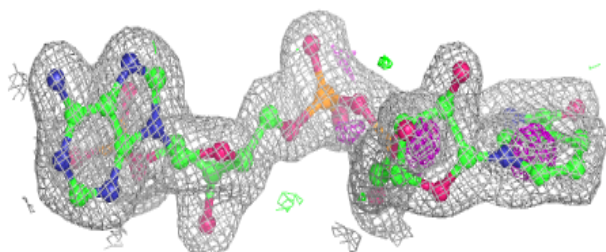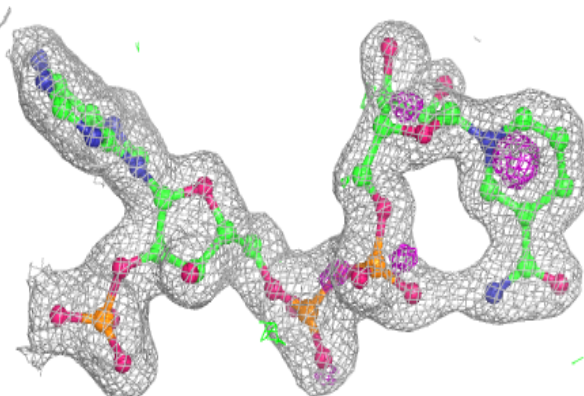
Electron density around NDP C 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
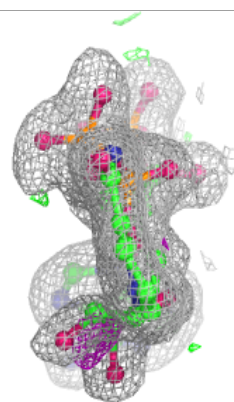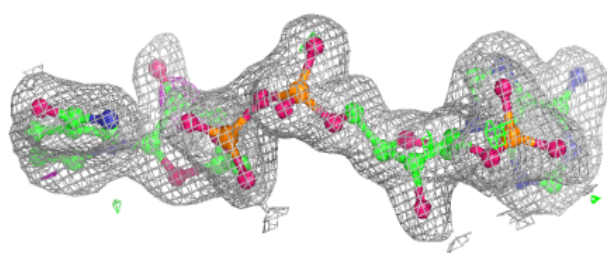
Electron density around NDP H 301:

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

Electron density around NDP D 301:

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 NDP E 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
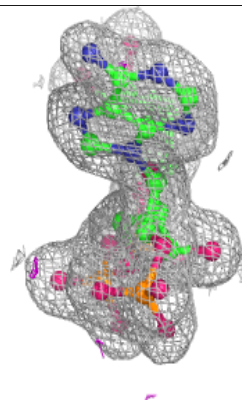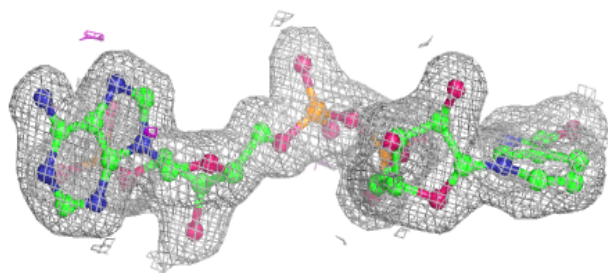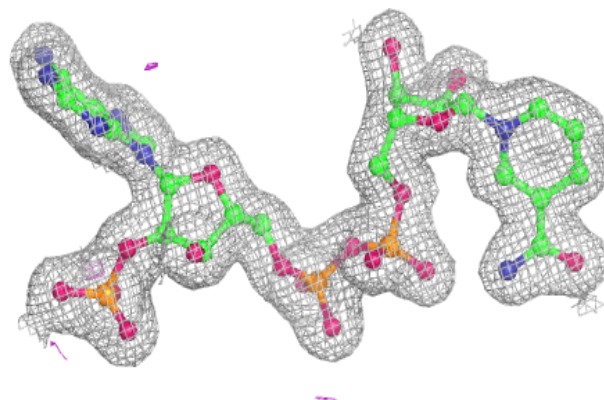
6.5 Other polymers (i)

There are no such residues in this entry.