Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 03:14 PM JST

PDB ID	:	6JHB
Title	:	Crystal structure of NADPH and 4-hydroxyphenylpyruvic acid bound AerF from Microcystis aeruginosa
Authors	:	Qiu, X.; Wei, Y.; Zhu, W.
Deposited on	:	2019-02-17
Resolution	:	2.27 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 (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:

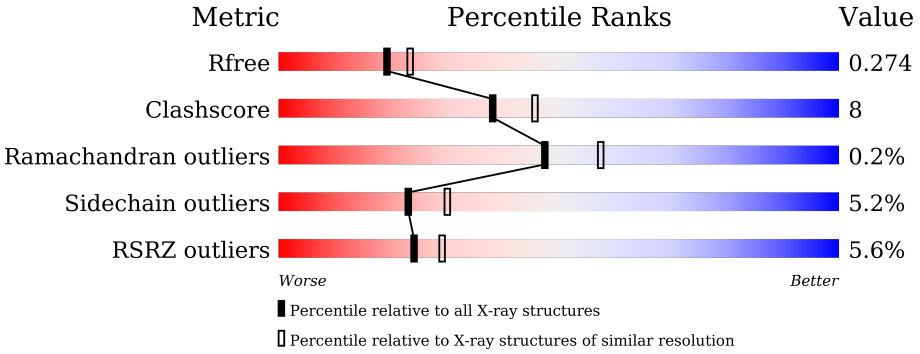
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.27 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	274	3% 72% 14% •• 13%
1	B	274	7% 80% 15% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3869 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.

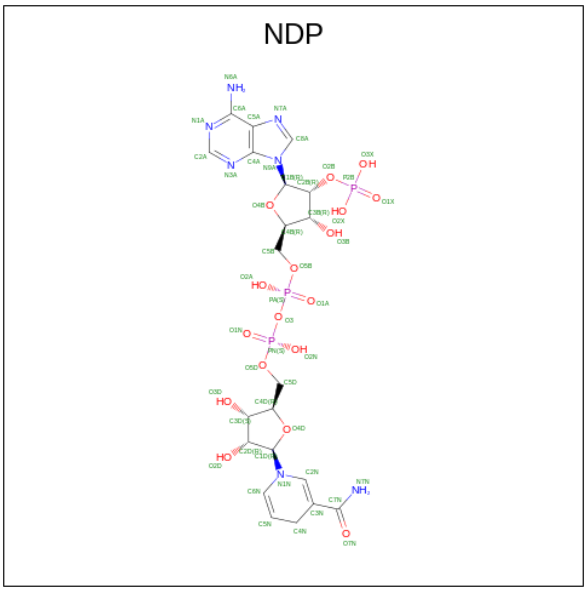
- Molecule 1 is a protein called Short chain dehydrogenase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	239	1749	1123	291	328	7	0	2	1
1	B	264	1958	1254	330	367	7	0	2	0

There are 16 discrepancies between the modelled and reference sequences:

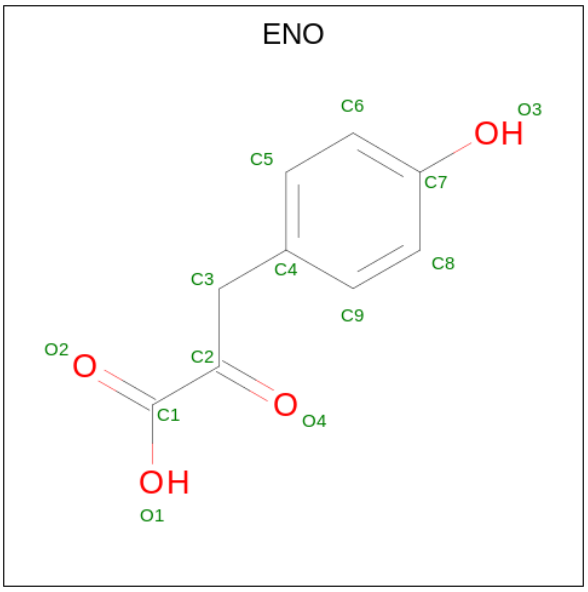
Chain	Residue	Modelled	Actual	Comment	Reference
A	267	LEU	-	expression tag	UNP L8NWH6
A	268	GLU	-	expression tag	UNP L8NWH6
A	269	HIS	-	expression tag	UNP L8NWH6
A	270	HIS	-	expression tag	UNP L8NWH6
A	271	HIS	-	expression tag	UNP L8NWH6
A	272	HIS	-	expression tag	UNP L8NWH6
A	273	HIS	-	expression tag	UNP L8NWH6
A	274	HIS	-	expression tag	UNP L8NWH6
B	267	LEU	-	expression tag	UNP L8NWH6
B	268	GLU	-	expression tag	UNP L8NWH6
B	269	HIS	-	expression tag	UNP L8NWH6
B	270	HIS	-	expression tag	UNP L8NWH6
B	271	HIS	-	expression tag	UNP L8NWH6
B	272	HIS	-	expression tag	UNP L8NWH6
B	273	HIS	-	expression tag	UNP L8NWH6
B	274	HIS	-	expression tag	UNP L8NWH6

- 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
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	B	1	48	21	7	17	3	0	0

- Molecule 3 is 3-(4-HYDROXY-PHENYL)PYRUVIC ACID (three-letter code: ENO) (formula: $C_9H_8O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	13	9	4	0	0

- Molecule 4 is water.

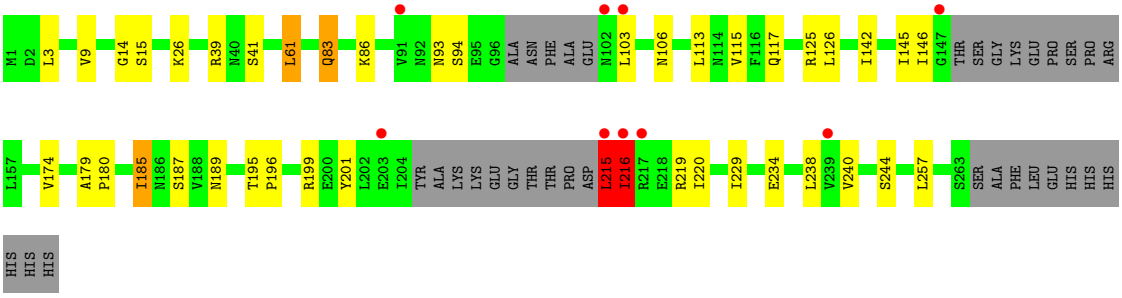
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	28	28	28	0	0
			Total	O		
4	B	25	25	25	0	0

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.

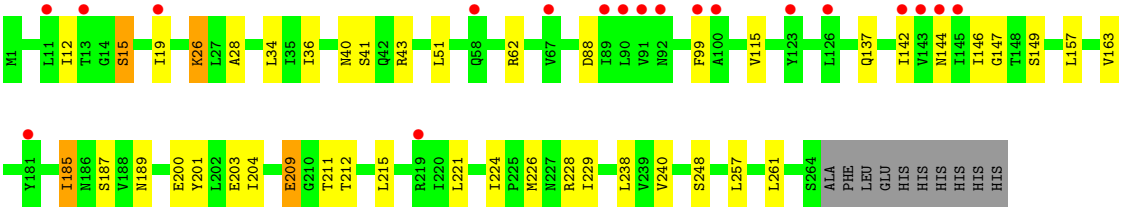
• Molecule 1: Short chain dehydrogenase family protein

Chain A:



• Molecule 1: Short chain dehydrogenase family protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	101.12Å 101.12Å 115.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.27 28.05 – 2.27	Depositor EDS
% Data completeness (in resolution range)	95.0 (45.00-2.27) 95.1 (28.05-2.27)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.68 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.239 , 0.270 0.243 , 0.274	Depositor DCC
R_{free} test set	1362 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3869	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NDP, ENO

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	1.53	2/1784 (0.1%)	0.76	3/2418 (0.1%)
1	B	3.03	2/1998 (0.1%)	1.33	6/2711 (0.2%)
All	All	2.44	4/3782 (0.1%)	1.10	9/5129 (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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209[A]	GLU	CG-CD	94.50	2.93	1.51
1	B	209[B]	GLU	CG-CD	94.50	2.93	1.51
1	A	216[A]	ILE	CG1-CD1	42.81	4.45	1.50
1	A	216[B]	ILE	CG1-CD1	42.81	4.45	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	209[A]	GLU	CG-CD-OE1	-26.59	65.12	118.30
1	B	209[B]	GLU	CG-CD-OE1	-26.59	65.12	118.30
1	B	209[A]	GLU	CG-CD-OE2	25.61	169.53	118.30
1	B	209[B]	GLU	CG-CD-OE2	25.61	169.53	118.30
1	B	209[A]	GLU	CB-CG-CD	-19.20	62.36	114.20
1	B	209[B]	GLU	CB-CG-CD	-19.20	62.36	114.20
1	A	216[A]	ILE	CB-CG1-CD1	-9.37	87.65	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216[B]	ILE	CB-CG1-CD1	-9.37	87.65	113.90
1	A	125	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	LEU	Peptide
1	A	216[B]	ILE	Peptide

5.2 Too-close contacts (i)

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	1749	0	1713	29	0
1	B	1958	0	1930	28	0
2	A	48	0	26	3	0
2	B	48	0	26	1	0
3	B	13	0	6	2	0
4	A	28	0	0	1	0
4	B	25	0	0	1	0
All	All	3869	0	3701	57	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 (57) 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:A:103:LEU:O	1:A:106:ASN:HB2	1.50	1.09
1:A:215:LEU:O	1:A:216[A]:ILE:HB	1.57	1.02
4:A:401:HOH:O	1:B:226:MET:HE1	1.76	0.85
1:A:215:LEU:HD13	1:A:215:LEU:N	1.95	0.81
1:A:103:LEU:O	1:A:106:ASN:CB	2.34	0.69
1:A:201:TYR:CG	1:A:201:TYR:O	2.48	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD23	1:A:257:LEU:HD12	1.77	0.65
1:B:211:THR:CG2	1:B:212:THR:N	2.60	0.65
1:B:142:ILE:HD12	1:B:185:ILE:HD13	1.80	0.64
1:A:145:ILE:HD13	1:A:145:ILE:N	2.16	0.59
1:B:211:THR:HG22	1:B:212:THR:N	2.17	0.59
1:B:203:GLU:HA	1:B:203:GLU:OE1	2.02	0.58
1:A:174:VAL:HG13	1:A:185:ILE:HG12	1.87	0.57
1:A:215:LEU:N	1:A:215:LEU:CD1	2.65	0.57
1:A:234:GLU:OE2	1:B:248:SER:OG	2.20	0.55
1:B:211:THR:CG2	1:B:212:THR:H	2.18	0.55
1:A:195:THR:HB	1:A:196:PRO:HD2	1.89	0.55
1:A:61:LEU:HG	1:A:83:GLN:HG3	1.87	0.55
1:B:99:PHE:CE2	1:B:201:TYR:HB2	2.43	0.53
1:A:14:GLY:HA2	2:A:301:NDP:H1B	1.91	0.53
1:B:12:ILE:O	1:B:15:SER:OG	2.23	0.52
1:A:195:THR:HB	1:A:196:PRO:CD	2.39	0.52
1:A:216[B]:ILE:HD12	1:A:219:ARG:HB2	1.91	0.52
1:B:149:SER:HB3	1:B:157:LEU:HD13	1.92	0.52
1:A:216[B]:ILE:CD1	1:A:219:ARG:HB2	2.40	0.52
1:A:9:VAL:HG23	1:A:86:LYS:HE3	1.91	0.52
1:A:94:SER:O	2:A:301:NDP:O3D	2.21	0.51
1:B:211:THR:HG23	1:B:212:THR:H	1.76	0.51
1:B:149:SER:HB3	3:B:302:ENO:O2	2.11	0.50
1:A:3:LEU:HB3	1:A:244:SER:HB2	1.93	0.50
1:A:216[B]:ILE:HD12	1:A:219:ARG:CB	2.41	0.50
2:B:301:NDP:H5N	3:B:302:ENO:O1	2.12	0.49
1:B:40:ASN:HB3	1:B:43[B]:ARG:HG2	1.95	0.49
1:A:113:LEU:O	1:A:117:GLN:HG3	2.14	0.48
1:B:146:ILE:HB	1:B:189:ASN:OD1	2.15	0.47
1:A:142:ILE:HB	1:A:185:ILE:HB	1.97	0.46
1:A:146:ILE:HD12	1:A:187:SER:HB3	1.99	0.45
1:B:26:LYS:HB3	1:B:240:VAL:HG21	1.99	0.45
1:A:103:LEU:HA	1:A:106:ASN:HD22	1.81	0.45
1:B:19:ILE:HG23	4:B:419:HOH:O	2.16	0.45
1:A:179:ALA:N	1:A:180:PRO:CD	2.79	0.44
1:A:93:ASN:OD1	2:A:301:NDP:H4D	2.18	0.44
1:B:238:LEU:HD23	1:B:257:LEU:HD12	1.99	0.44
1:B:200:GLU:O	1:B:204:ILE:HG23	2.16	0.44
1:B:28:ALA:HB2	1:B:34:LEU:HD11	2.00	0.44
1:B:224:ILE:HG12	1:B:261:LEU:HD13	1.99	0.44
1:A:196:PRO:HA	1:A:199:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:HD22	1:B:228:ARG:HA	2.02	0.42
1:A:26:LYS:HB3	1:A:240:VAL:HG21	2.01	0.41
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.91	0.41
1:B:36:ILE:HD13	1:B:51:LEU:CD1	2.50	0.41
1:B:88:ASP:OD1	1:B:137:GLN:NE2	2.53	0.41
1:B:144:ASN:HB2	1:B:187:SER:OG	2.20	0.41
1:B:142:ILE:HD12	1:B:185:ILE:CD1	2.50	0.41
1:B:146:ILE:HG22	1:B:147:GLY:N	2.36	0.41
1:B:115:VAL:HG12	1:B:163:VAL:CG2	2.51	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	233/274 (85%)	221 (95%)	10 (4%)	2 (1%)	17 18
1	B	264/274 (96%)	252 (96%)	12 (4%)	0	100 100
All	All	497/548 (91%)	473 (95%)	22 (4%)	2 (0%)	47 40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216[A]	ILE
1	A	216[B]	ILE

5.3.2 Protein sidechains (i)

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	173/233 (74%)	160 (92%)	13 (8%)	13	16
1	B	197/233 (84%)	190 (96%)	7 (4%)	35	47
All	All	370/466 (79%)	350 (95%)	20 (5%)	23	28

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	39	ARG
1	A	41	SER
1	A	61	LEU
1	A	83	GLN
1	A	115	VAL
1	A	185	ILE
1	A	189	ASN
1	A	215	LEU
1	A	216[A]	ILE
1	A	216[B]	ILE
1	A	220	ILE
1	A	229	ILE
1	B	15	SER
1	B	26	LYS
1	B	41	SER
1	B	62	ARG
1	B	185	ILE
1	B	215	LEU
1	B	229	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ENO	B	302	-	13,13,13	1.24	1 (7%)	17,17,17	2.01	6 (35%)
2	NDP	A	301	-	45,52,52	1.11	4 (8%)	53,80,80	1.26	8 (15%)
2	NDP	B	301	-	45,52,52	0.95	1 (2%)	53,80,80	1.18	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ENO	B	302	-	-	3/8/8/8	0/1/1/1
2	NDP	A	301	-	-	6/30/77/77	0/5/5/5
2	NDP	B	301	-	-	6/30/77/77	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NDP	C6N-C5N	3.82	1.40	1.33
3	B	302	ENO	C2-C1	-3.67	1.48	1.53
2	B	301	NDP	C6N-C5N	3.43	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NDP	C2A-N3A	2.97	1.36	1.32
2	A	301	NDP	C5A-C4A	2.39	1.47	1.40
2	A	301	NDP	O4B-C1B	2.38	1.44	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302	ENO	O1-C1-C2	4.23	125.53	113.97
2	A	301	NDP	N3A-C2A-N1A	-3.63	123.00	128.68
3	B	302	ENO	O2-C1-C2	-3.52	117.02	121.72
3	B	302	ENO	C4-C3-C2	3.32	117.95	113.64
2	B	301	NDP	N3A-C2A-N1A	-3.20	123.68	128.68
2	B	301	NDP	C4A-C5A-N7A	-3.09	106.17	109.40
3	B	302	ENO	O1-C1-O2	-2.69	117.45	123.61
2	A	301	NDP	C4A-C5A-N7A	-2.51	106.78	109.40
2	A	301	NDP	PN-O3-PA	-2.49	124.27	132.83
2	A	301	NDP	C1D-N1N-C2N	-2.42	117.09	121.11
3	B	302	ENO	O4-C2-C1	2.41	122.93	119.43
2	A	301	NDP	N6A-C6A-N1A	2.37	123.48	118.57
2	B	301	NDP	PN-O3-PA	-2.17	125.37	132.83
2	A	301	NDP	O2B-P2B-O1X	-2.09	101.32	109.39
3	B	302	ENO	O4-C2-C3	-2.09	116.46	120.84
2	A	301	NDP	O7N-C7N-C3N	-2.07	117.00	120.90
2	A	301	NDP	O2A-PA-O1A	2.02	122.20	112.24

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NDP	C5D-O5D-PN-O1N
2	A	301	NDP	C5D-O5D-PN-O2N
2	B	301	NDP	C2B-O2B-P2B-O3X
2	B	301	NDP	C5D-O5D-PN-O1N
3	B	302	ENO	O2-C1-C2-O4
3	B	302	ENO	O2-C1-C2-C3
3	B	302	ENO	O1-C1-C2-C3
2	A	301	NDP	O4D-C1D-N1N-C6N
2	B	301	NDP	O4D-C1D-N1N-C6N
2	B	301	NDP	C5D-O5D-PN-O3
2	B	301	NDP	C5D-O5D-PN-O2N
2	B	301	NDP	O4B-C4B-C5B-O5B
2	A	301	NDP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
2	A	301	NDP	O4B-C4B-C5B-O5B
2	A	301	NDP	C1B-C2B-O2B-P2B

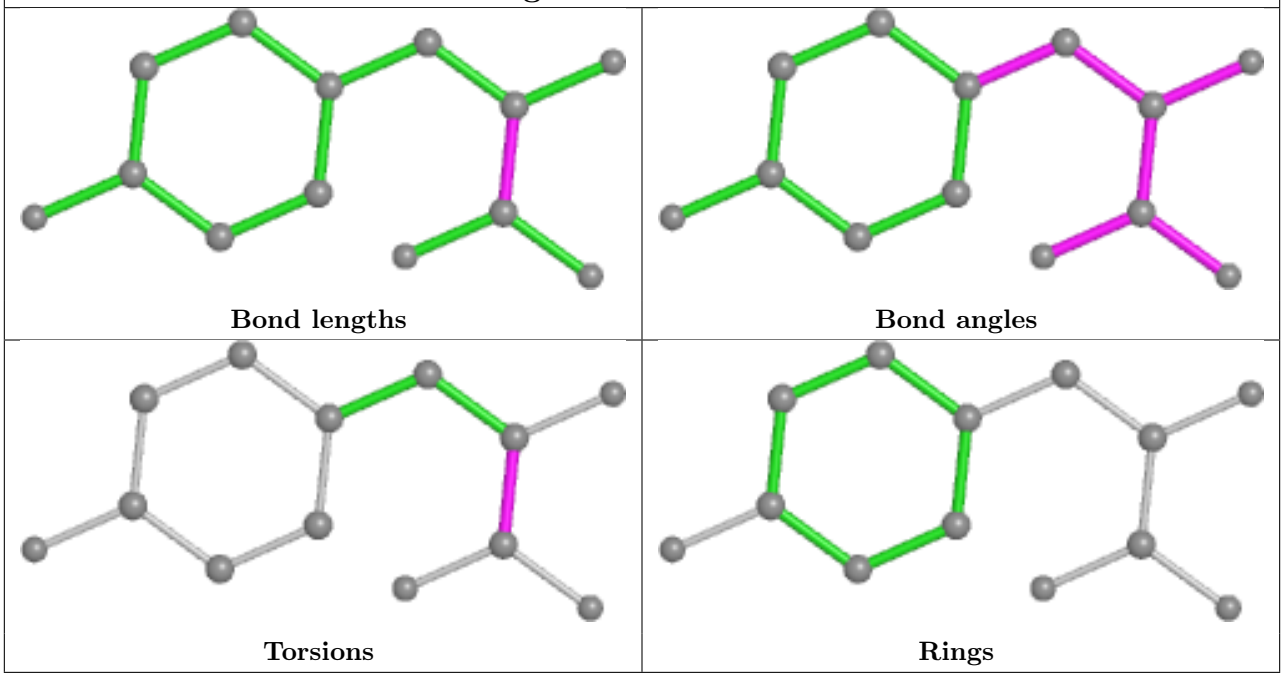
There are no ring outliers.

3 monomers are involved in 5 short contacts:

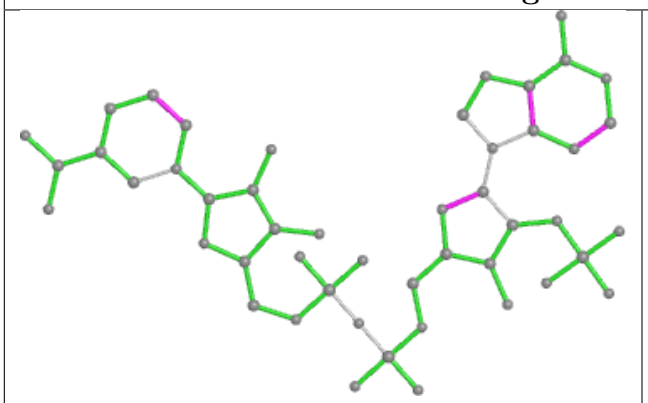
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	ENO	2	0
2	A	301	NDP	3	0
2	B	301	NDP	1	0

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.

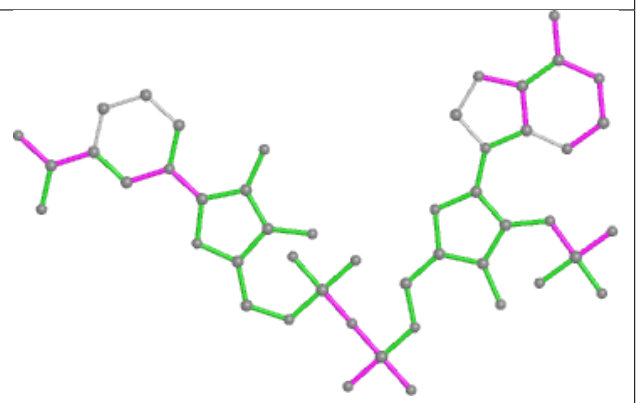
Ligand ENO B 302



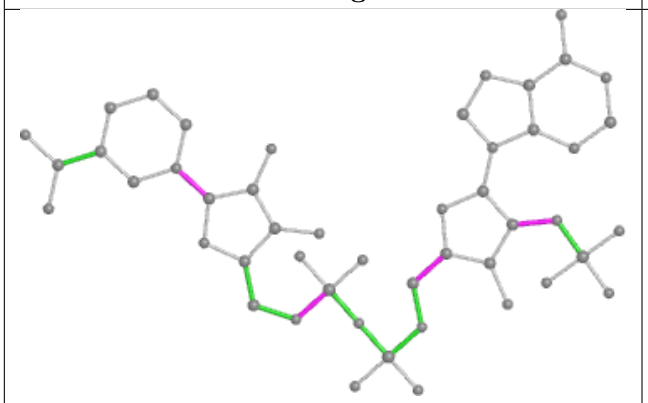
Ligand NDP A 301



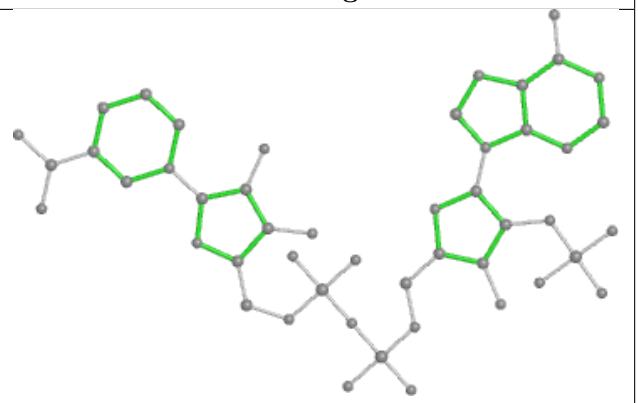
Bond lengths



Bond angles

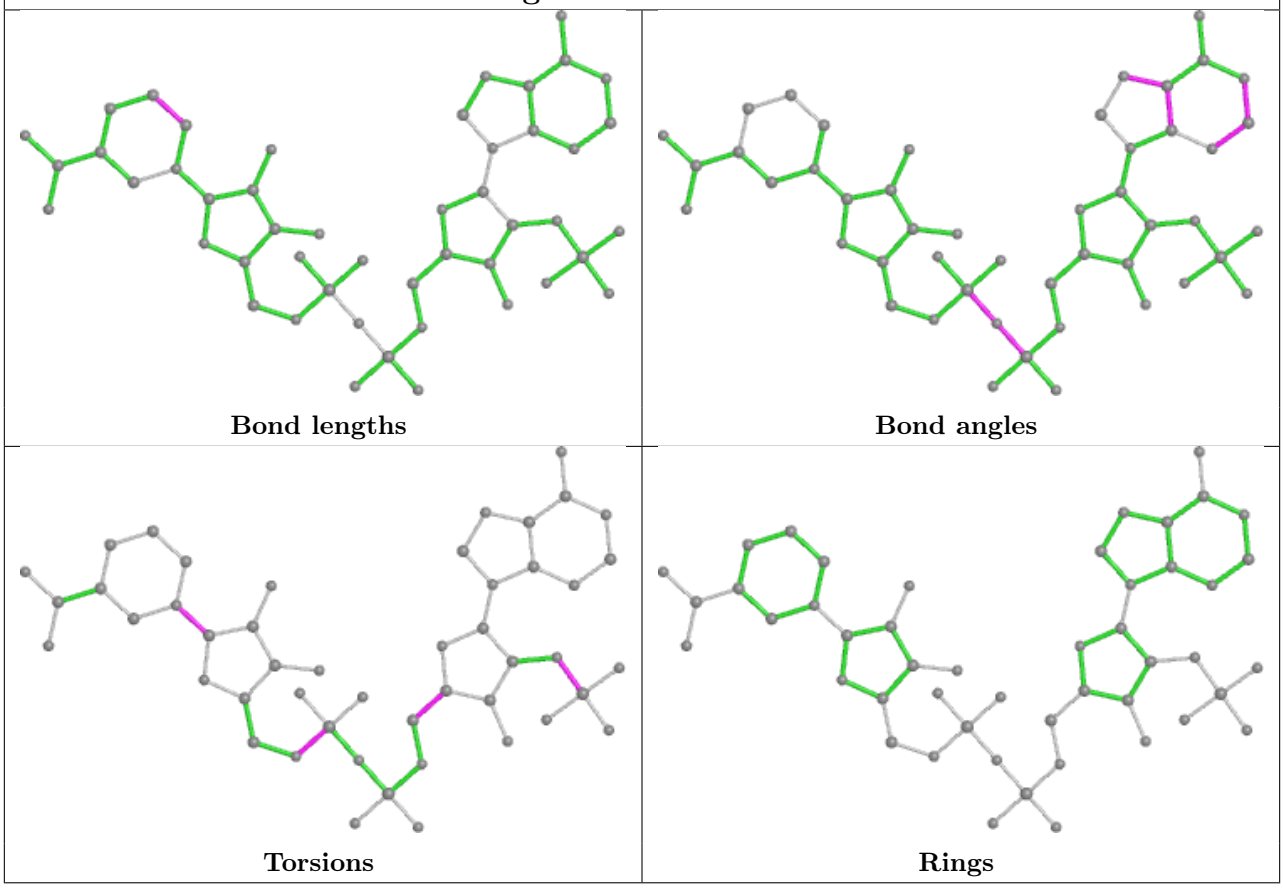


Torsions



Rings

Ligand NDP B 301



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	239/274 (87%)	0.13	9 (3%)	40	45	31, 42, 64, 87	2 (0%)
1	B	264/274 (96%)	0.28	19 (7%)	15	19	32, 42, 64, 76	5 (1%)
All	All	503/548 (91%)	0.21	28 (5%)	24	29	31, 42, 64, 87	7 (1%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	LEU	4.2
1	A	102	ASN	4.1
1	A	215	LEU	3.8
1	B	100	ALA	3.8
1	B	91	VAL	3.6
1	B	126	LEU	3.5
1	B	92	ASN	3.4
1	A	147	GLY	3.4
1	A	91	VAL	3.0
1	A	203	GLU	2.8
1	B	219	ARG	2.8
1	B	144	ASN	2.7
1	B	143	VAL	2.7
1	B	58	GLN	2.6
1	B	145	ILE	2.6
1	A	103	LEU	2.6
1	B	13	THR	2.5
1	B	142	ILE	2.5
1	B	123	TYR	2.5
1	B	99	PHE	2.4
1	B	89	ILE	2.4
1	A	239	VAL	2.3
1	A	216[A]	ILE	2.3
1	B	67	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	19	ILE	2.2
1	B	181	TYR	2.1
1	A	217	ARG	2.1
1	B	11	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

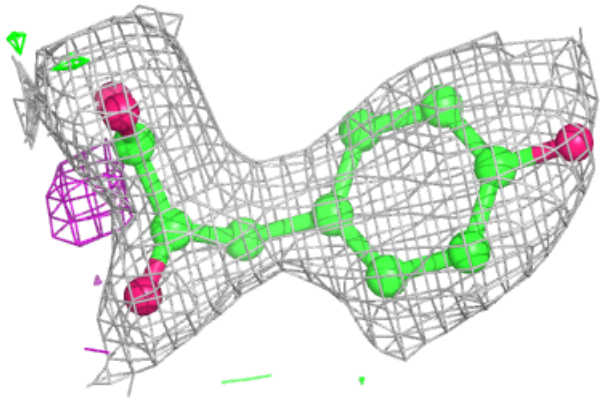
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

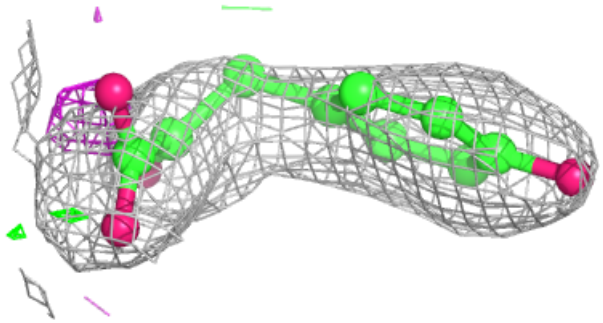
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ENO	B	302	13/13	0.83	0.23	56,60,65,75	0
2	NDP	A	301	48/48	0.86	0.17	49,64,71,75	0
2	NDP	B	301	48/48	0.95	0.11	36,41,47,48	0

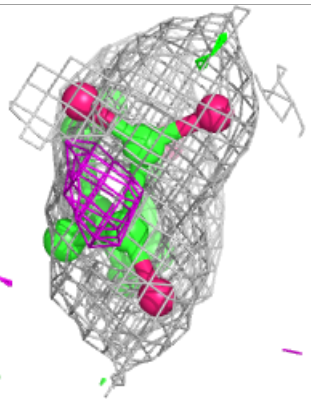
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ENO B 302:

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

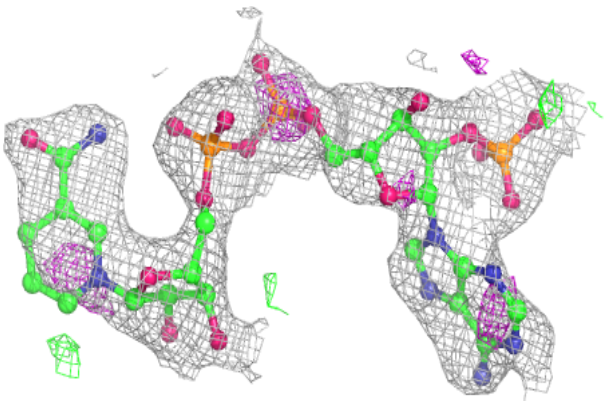


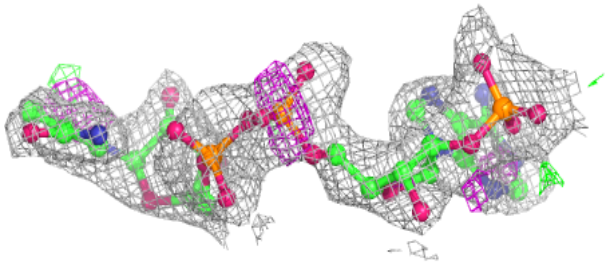


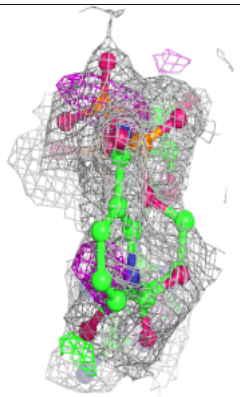


Electron density around NDP A 301:

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

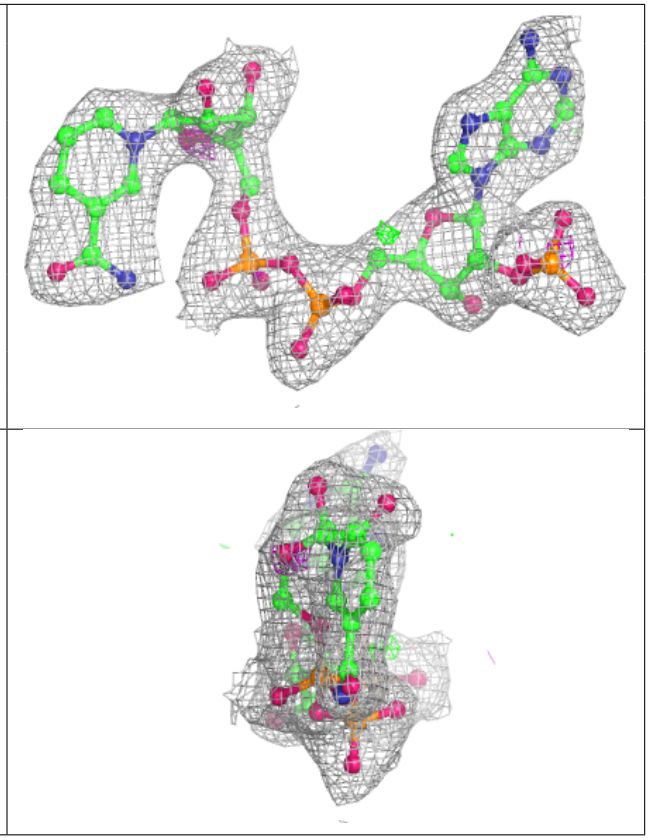






Electron density around NDP B 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.