wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2023 – 10:57 AM EDT

PDB ID	:	3INM
Title	:	Crystal structure of human cytosolic NADP(+)-dependent isocitrate dehydrogenase R132H mutant in complex with NADPH, ALPHA-KETOGLUTARATE and CALCIUM(2+)
Authors	:	Fontano, E.; Brown, R.S.; Suto, R.K.; Bhyravbhatla, B.
Deposited on	:	2009-08-12
Resolution	:	2.10 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:

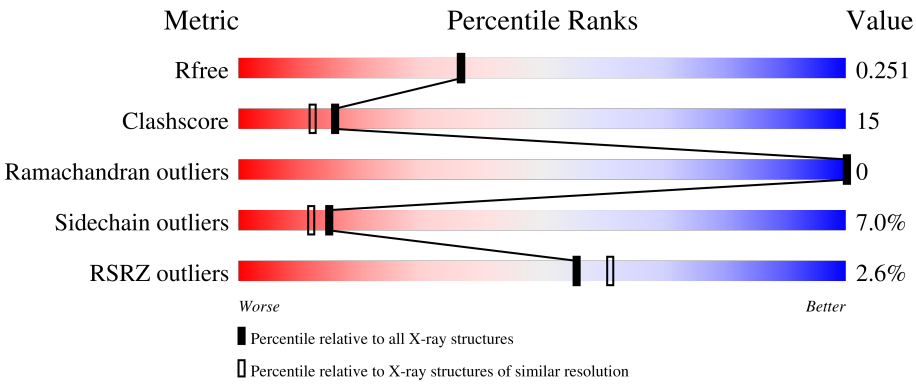
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	425	3% 73% 22% • •
1	B	425	% 75% 19% • •
1	C	425	3% 67% 26% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	531	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10205 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	407	3225	2051	545	611	18	0	0	0
1	B	411	3256	2071	551	616	18	0	0	0
1	C	407	3225	2051	545	611	18	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	HIS	ARG	engineered mutation	UNP O75874
A	415	SER	-	expression tag	UNP O75874
A	416	LEU	-	expression tag	UNP O75874
A	417	GLU	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag	UNP O75874
A	423	HIS	-	expression tag	UNP O75874
A	424	HIS	-	expression tag	UNP O75874
A	425	HIS	-	expression tag	UNP O75874
B	132	HIS	ARG	engineered mutation	UNP O75874
B	415	SER	-	expression tag	UNP O75874
B	416	LEU	-	expression tag	UNP O75874
B	417	GLU	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874
B	419	HIS	-	expression tag	UNP O75874
B	420	HIS	-	expression tag	UNP O75874
B	421	HIS	-	expression tag	UNP O75874
B	422	HIS	-	expression tag	UNP O75874
B	423	HIS	-	expression tag	UNP O75874
B	424	HIS	-	expression tag	UNP O75874

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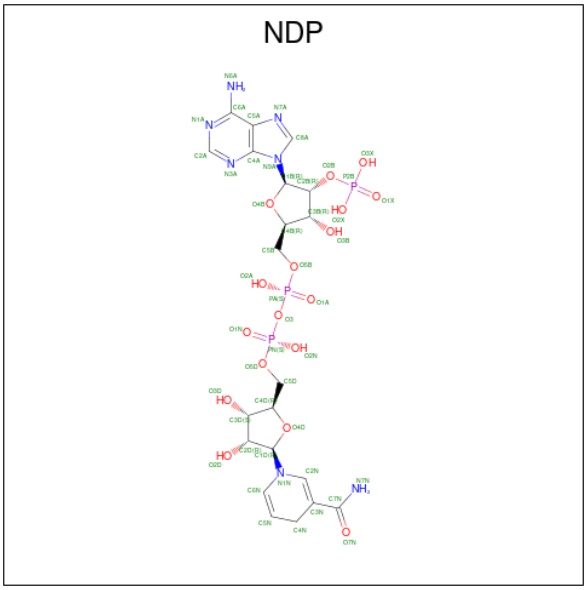
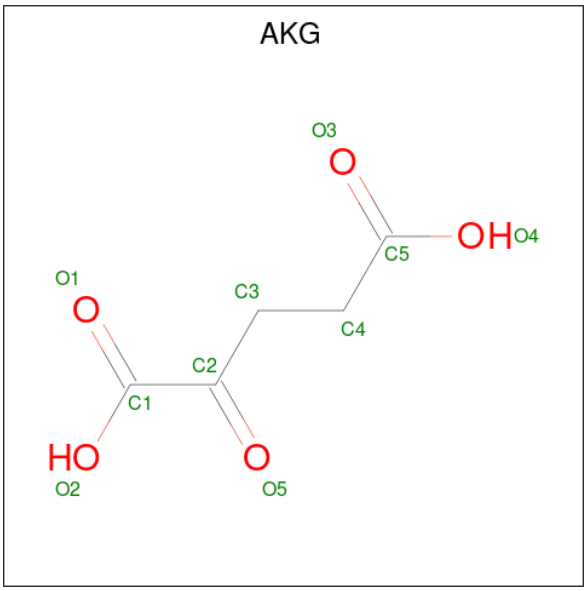
Chain	Residue	Modelled	Actual	Comment	Reference
B	425	HIS	-	expression tag	UNP O75874
C	132	HIS	ARG	engineered mutation	UNP O75874
C	415	SER	-	expression tag	UNP O75874
C	416	LEU	-	expression tag	UNP O75874
C	417	GLU	-	expression tag	UNP O75874
C	418	HIS	-	expression tag	UNP O75874
C	419	HIS	-	expression tag	UNP O75874
C	420	HIS	-	expression tag	UNP O75874
C	421	HIS	-	expression tag	UNP O75874
C	422	HIS	-	expression tag	UNP O75874
C	423	HIS	-	expression tag	UNP O75874
C	424	HIS	-	expression tag	UNP O75874
C	425	HIS	-	expression tag	UNP O75874

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 5	0	0
3	B	1	Total C O 10 5 5	0	0
3	C	1	Total C O 10 5 5	0	0

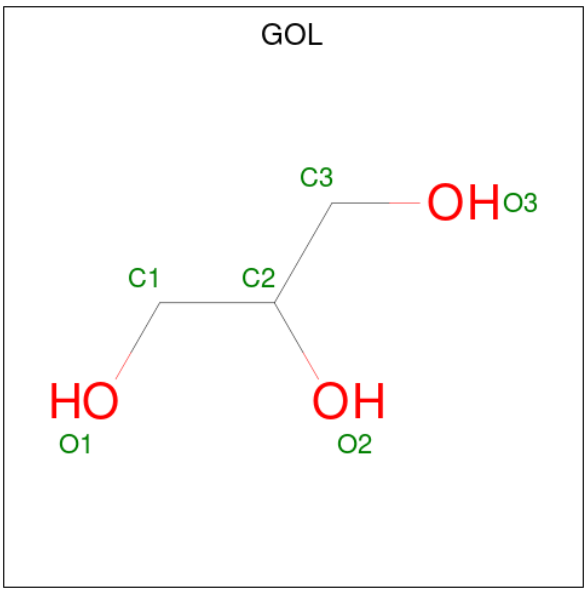
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	C	1	6	3	3	0	0

- Molecule 7 is water.

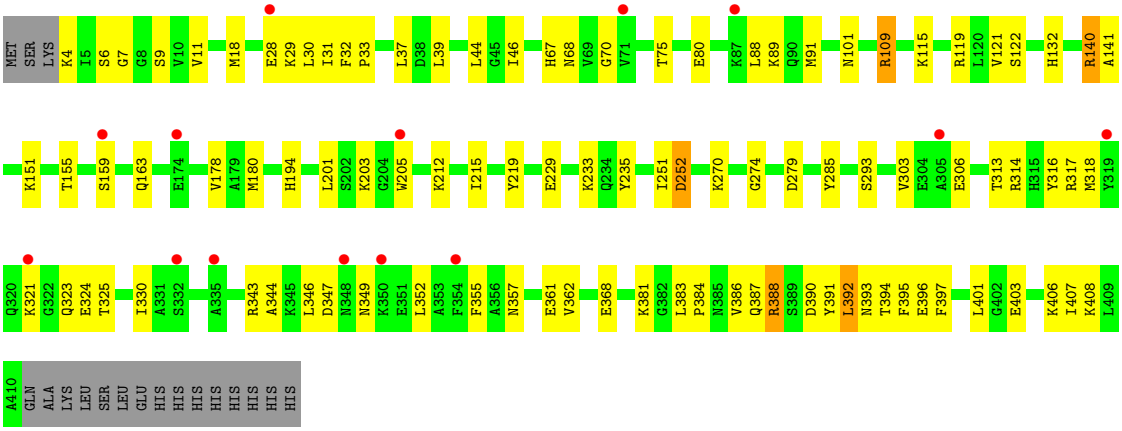
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	112	112	112	0	0
			Total	O		
7	B	112	112	112	0	0
			Total	O		
7	C	77	77	77	0	0

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.

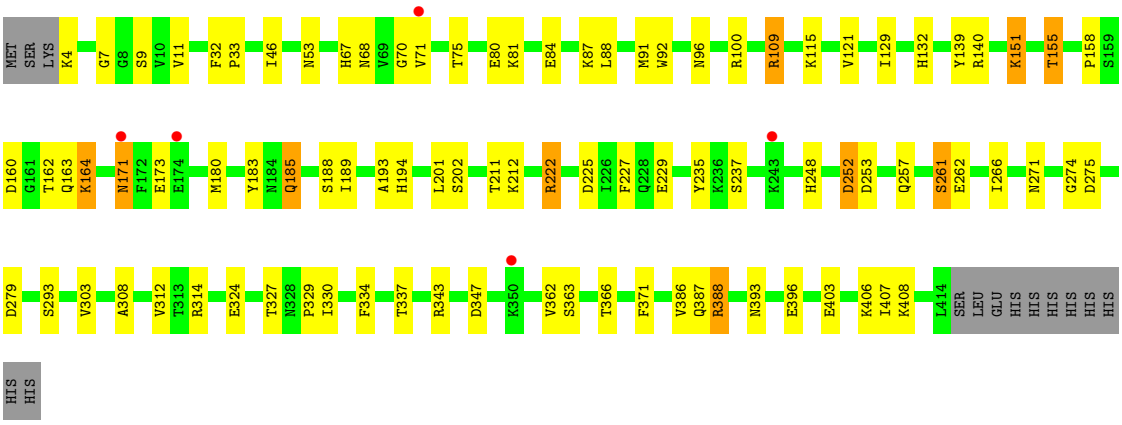
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain A:



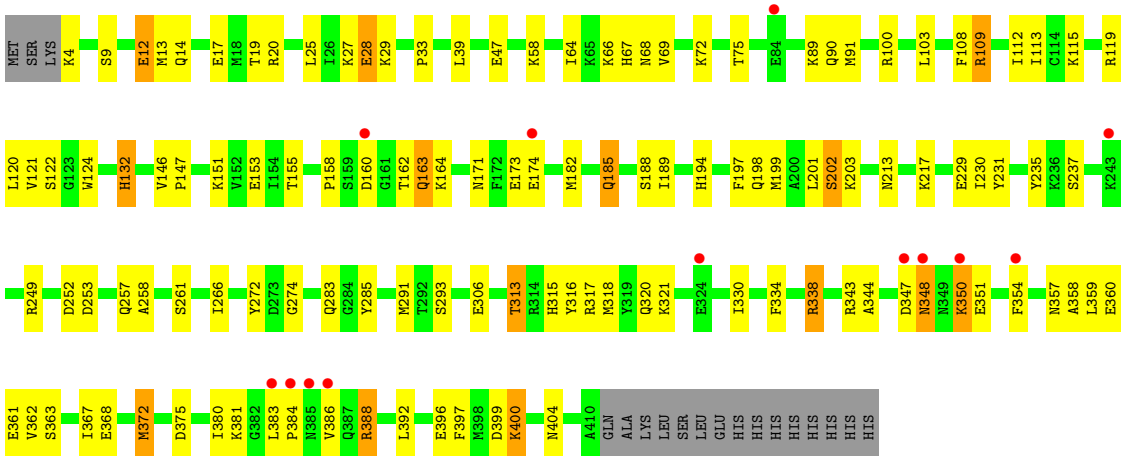
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain B:



• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain C:


MET SER LYS K4 S9 E12 M13 Q14 E17 M18 T19 R20 L25 I26 K27 E28 K29 P33 L39 E47 K58 I64 K65 K66 H67 N68 V69 K72 T75 E84 K89 Q90 M91 R100 L103 F108 R109 I112 I113 C114 K115 R119
L120 V121 S122 G123 W124 H132 V146 P147 K151 V152 E153 I154 T155 P158 S159 D160 G161 T162 Q163 K164 N171 F172 E173 E174 M182 Q185 S188 I189 H194 F197 Q198 M199 A200 L201 S202 K203 N213 K217 E229 I230 Y231 Y235 K236 S237 K243
R249 D252 D253 Q257 A258 S261 I266 Y272 D273 G274 Q283 G284 Y285 M291 T292 S293 E306 T313 R314 H315 Y316 R317 M318 Y319 Q320 K321 E324 I330 F334 R338 R343 A344 D347 N348 M349 K350 E351 F354 N357 A358 L359 E360
E361 V362 S363 I367 E368 M372 D375 I380 K381 G382 L383 P384 N385 V386 Q387 R388 L392 E396 F397 M398 D399 K400 N404 A410 GLN ALA LYS LEU SER LEU GLU HIS HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	96.12Å 274.69Å 116.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.91 – 2.10 24.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.4 (24.91-2.10) 92.4 (24.91-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.262 0.215 , 0.251	Depositor DCC
R_{free} test set	4153 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10205	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: CA, NDP, NA, AKG, GOL

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	0.70	0/3294	0.55	0/4444
1	B	0.79	1/3325 (0.0%)	0.58	1/4485 (0.0%)
1	C	0.80	3/3294 (0.1%)	0.57	0/4444
All	All	0.76	4/9913 (0.0%)	0.57	1/13373 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	69	VAL	CB-CG2	-5.79	1.40	1.52
1	C	174	GLU	CB-CG	5.55	1.62	1.52
1	B	262	GLU	CG-CD	5.10	1.59	1.51
1	C	272	TYR	CD1-CE1	-5.08	1.31	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	7	GLY	N-CA-C	5.40	126.60	113.10

There are no chirality outliers.

There are no planarity outliers.

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	3225	0	3183	85	0
1	B	3256	0	3220	71	0
1	C	3225	0	3183	134	0
2	A	48	0	26	1	0
2	B	48	0	26	5	0
2	C	48	0	26	4	0
3	A	10	0	4	0	0
3	B	10	0	4	1	0
3	C	10	0	4	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	12	0	16	13	0
6	C	6	0	8	2	0
7	A	112	0	0	1	0
7	B	112	0	0	1	0
7	C	77	0	0	7	0
All	All	10205	0	9700	286	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 15.

The worst 5 of 286 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:395:PHE:CD1	6:A:531:GOL:H12	1.46	1.47
1:C:388:ARG:O	1:C:388:ARG:HD3	1.20	1.32
1:A:388:ARG:HD2	1:A:388:ARG:O	1.16	1.29
1:A:395:PHE:HD1	6:A:531:GOL:C1	1.47	1.26
1:B:388:ARG:CD	1:B:388:ARG:O	1.89	1.21

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	405/425 (95%)	391 (96%)	14 (4%)	0	100	100
1	B	409/425 (96%)	399 (98%)	10 (2%)	0	100	100
1	C	405/425 (95%)	388 (96%)	17 (4%)	0	100	100
All	All	1219/1275 (96%)	1178 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	344/361 (95%)	323 (94%)	21 (6%)	18	16
1	B	347/361 (96%)	322 (93%)	25 (7%)	14	11
1	C	344/361 (95%)	318 (92%)	26 (8%)	13	10
All	All	1035/1083 (96%)	963 (93%)	72 (7%)	15	12

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	185	GLN
1	C	400	LYS
1	C	202	SER
1	C	348	ASN
1	B	109	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	323	GLN
1	C	277	GLN
1	C	90	GLN
1	C	194	HIS
1	B	323	GLN

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)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	NDP	C	501	-	45,52,52	1.38	4 (8%)	53,80,80	1.23	2 (3%)
3	AKG	A	511	-	9,9,9	2.17	1 (11%)	11,11,11	1.53	2 (18%)
2	NDP	B	501	-	45,52,52	1.53	4 (8%)	53,80,80	1.06	1 (1%)
3	AKG	B	511	-	9,9,9	1.85	1 (11%)	11,11,11	1.46	2 (18%)
6	GOL	A	532	-	5,5,5	0.43	0	5,5,5	0.62	0
6	GOL	A	531	-	5,5,5	0.49	0	5,5,5	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	GOL	C	532	-	5,5,5	0.68	0	5,5,5	0.69	0
2	NDP	A	501	-	45,52,52	1.51	5 (11%)	53,80,80	1.11	2 (3%)
3	AKG	C	511	-	9,9,9	1.82	1 (11%)	11,11,11	1.60	2 (18%)

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	C	501	-	-	9/30/77/77	0/5/5/5
3	AKG	A	511	-	-	2/9/9/9	-
2	NDP	B	501	-	-	8/30/77/77	0/5/5/5
3	AKG	B	511	-	-	2/9/9/9	-
6	GOL	A	532	-	-	2/4/4/4	-
6	GOL	A	531	-	-	0/4/4/4	-
6	GOL	C	532	-	-	1/4/4/4	-
2	NDP	A	501	-	-	10/30/77/77	0/5/5/5
3	AKG	C	511	-	-	0/9/9/9	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NDP	O7N-C7N	6.52	1.39	1.24
2	A	501	NDP	O7N-C7N	6.03	1.38	1.24
3	A	511	AKG	C2-C1	-5.78	1.45	1.53
2	C	501	NDP	O7N-C7N	5.75	1.38	1.24
3	B	511	AKG	C2-C1	-4.55	1.47	1.53

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	NDP	N3A-C2A-N1A	-5.88	119.48	128.68
2	B	501	NDP	N3A-C2A-N1A	-5.43	120.19	128.68
2	A	501	NDP	N3A-C2A-N1A	-5.33	120.35	128.68
2	A	501	NDP	C1D-N1N-C2N	-3.15	115.87	121.11
3	C	511	AKG	C3-C4-C5	-3.00	107.15	113.60

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NDP	C5B-O5B-PA-O3
2	A	501	NDP	PA-O3-PN-O5D
2	A	501	NDP	C5D-O5D-PN-O2N
2	B	501	NDP	C5B-O5B-PA-O3
2	B	501	NDP	PA-O3-PN-O5D

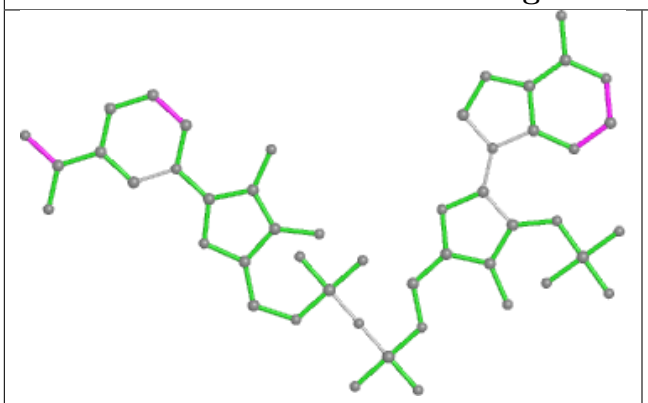
There are no ring outliers.

7 monomers are involved in 26 short contacts:

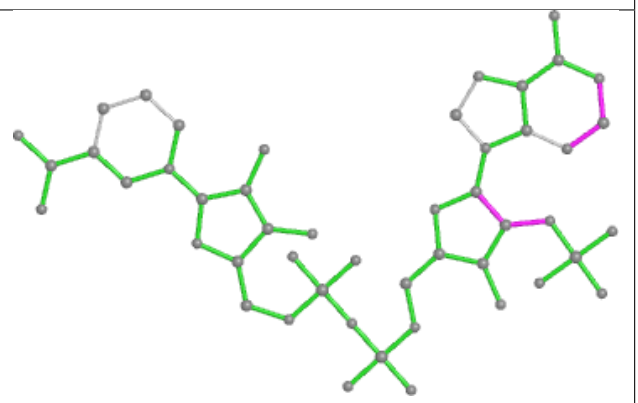
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NDP	4	0
2	B	501	NDP	5	0
3	B	511	AKG	1	0
6	A	531	GOL	13	0
6	C	532	GOL	2	0
2	A	501	NDP	1	0
3	C	511	AKG	2	0

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.

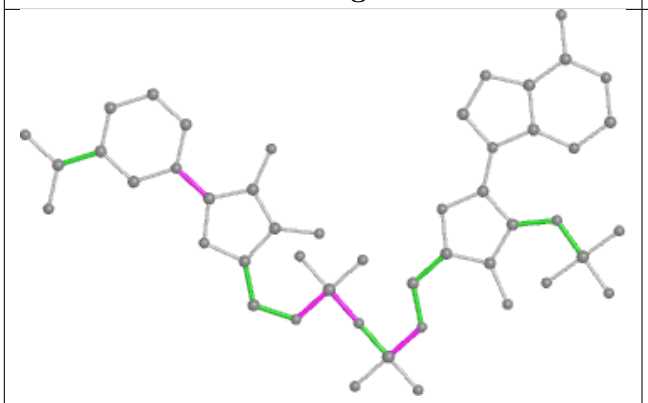
Ligand NDP C 501



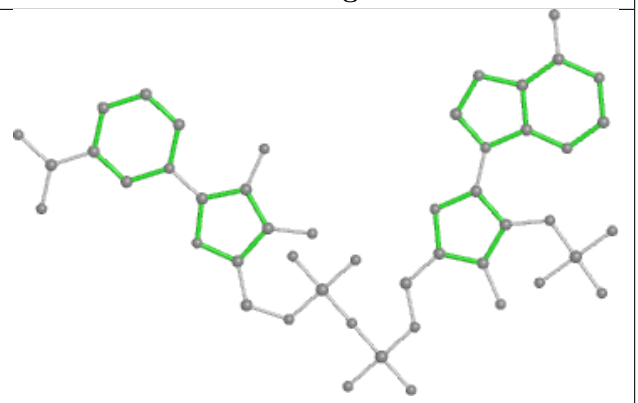
Bond lengths



Bond angles

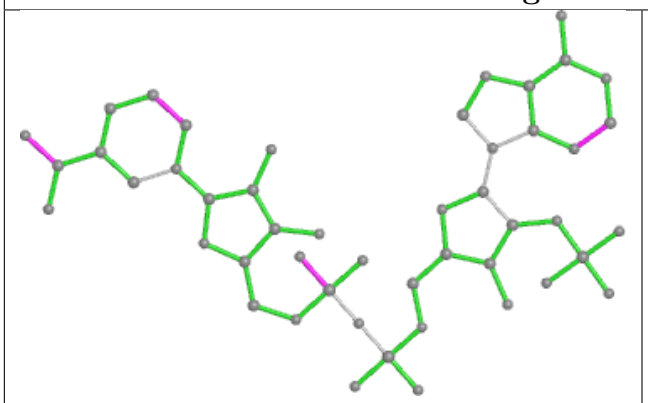


Torsions

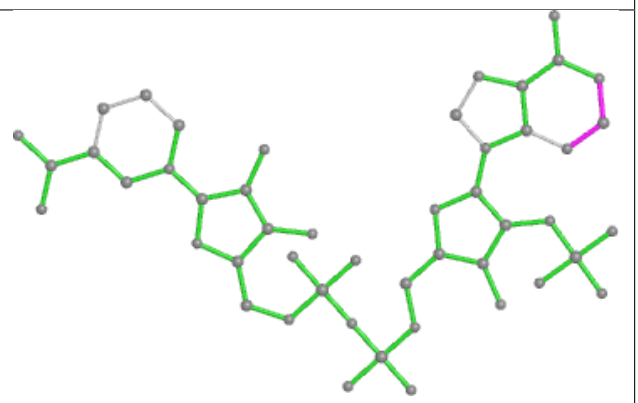


Rings

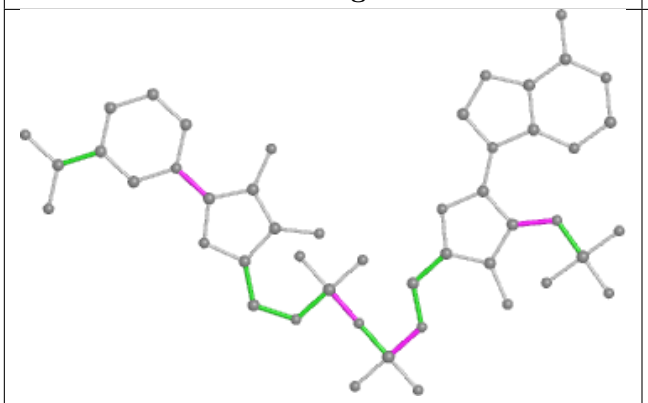
Ligand NDP B 501



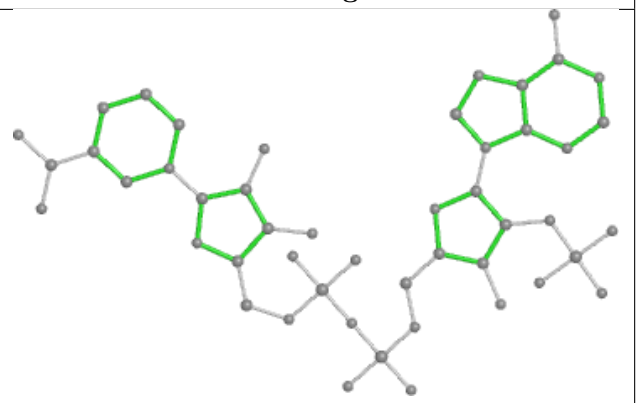
Bond lengths



Bond angles

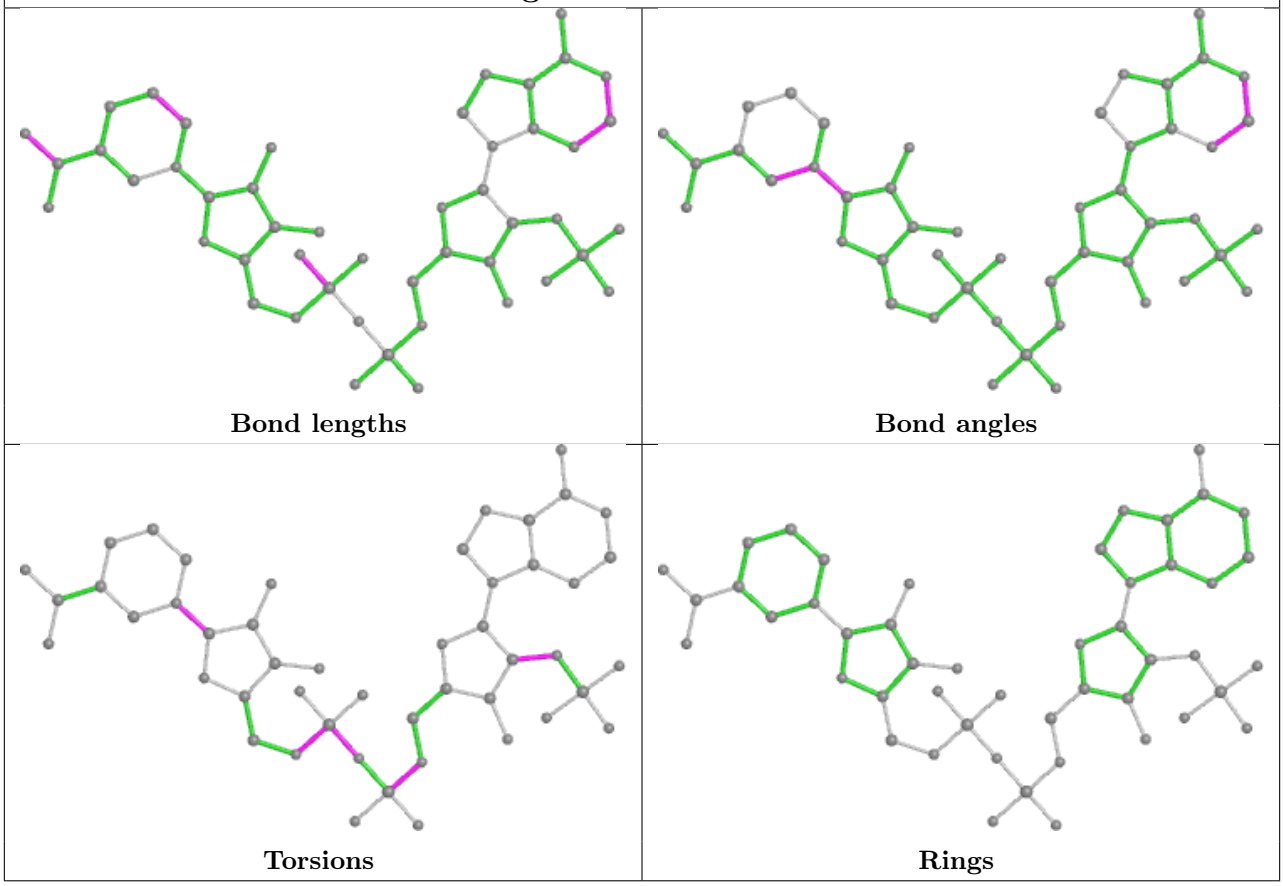


Torsions



Rings

Ligand NDP A 501



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	407/425 (95%)	0.16	14 (3%)	45	51	19, 32, 45, 54	0
1	B	411/425 (96%)	0.04	5 (1%)	79	82	19, 29, 42, 50	0
1	C	407/425 (95%)	0.26	13 (3%)	47	54	23, 34, 49, 59	0
All	All	1225/1275 (96%)	0.15	32 (2%)	56	61	19, 32, 45, 59	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	174	GLU	4.0
1	A	71	VAL	3.3
1	A	205	TRP	3.2
1	C	383	LEU	3.1
1	C	354	PHE	2.9

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)

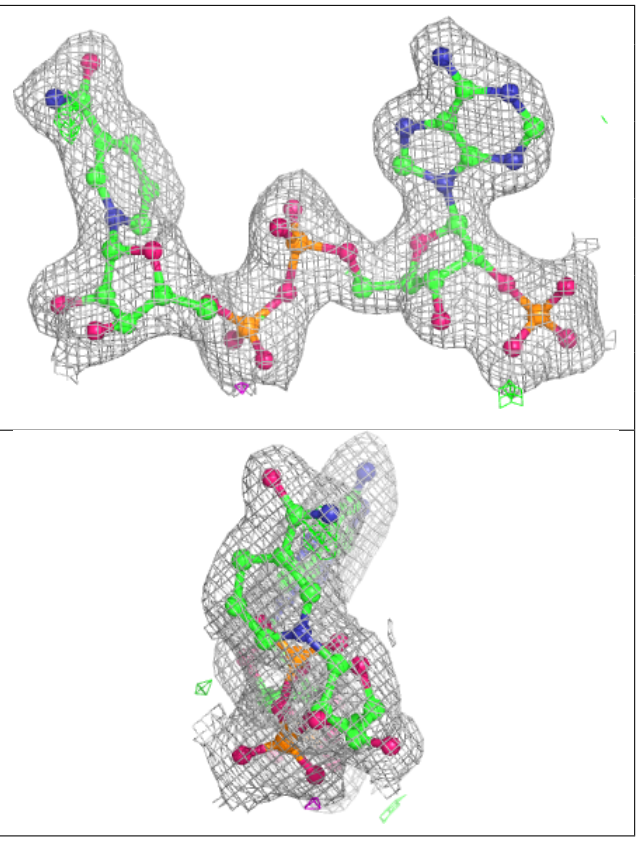
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	C	532	6/6	0.76	0.30	32,34,35,36	0
6	GOL	A	531	6/6	0.79	0.40	29,34,36,37	0
6	GOL	A	532	6/6	0.85	0.26	28,33,36,43	0
5	NA	B	522	1/1	0.88	0.14	30,30,30,30	0
3	AKG	C	511	10/10	0.89	0.15	38,44,48,49	0
3	AKG	A	511	10/10	0.92	0.14	35,41,45,47	0
3	AKG	B	511	10/10	0.93	0.14	32,37,41,45	0
5	NA	C	522	1/1	0.95	0.11	30,30,30,30	0
5	NA	A	522	1/1	0.95	0.09	30,30,30,30	0
2	NDP	A	501	48/48	0.96	0.12	20,28,36,40	0
2	NDP	C	501	48/48	0.97	0.12	22,29,34,37	0
2	NDP	B	501	48/48	0.97	0.11	19,24,32,37	0
4	CA	A	521	1/1	0.97	0.04	35,35,35,35	0
4	CA	B	521	1/1	0.98	0.08	33,33,33,33	0
4	CA	C	521	1/1	0.99	0.12	41,41,41,41	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.

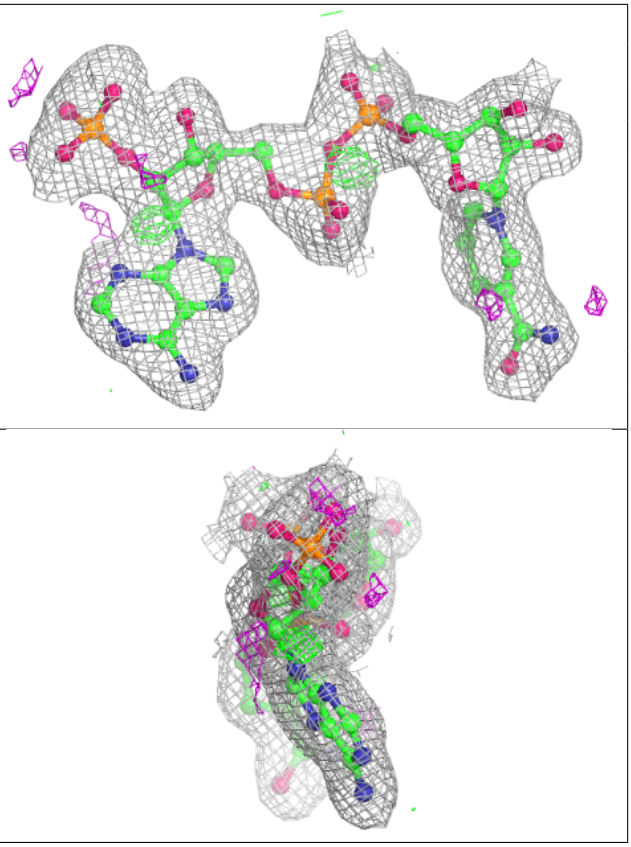
Electron density around NDP A 501:

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



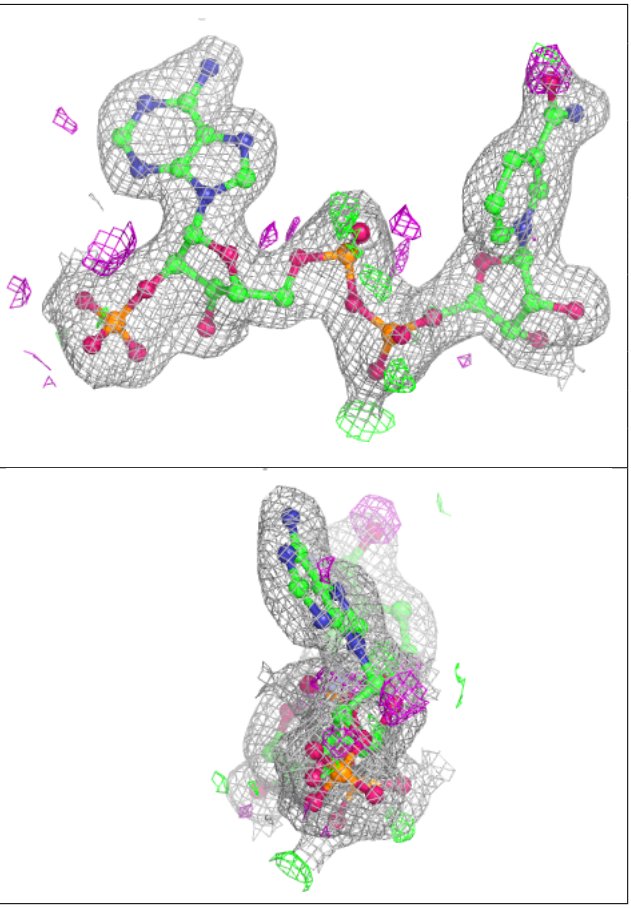
Electron density around NDP C 501:

$2mF_o$-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 501:

$2mF_o$-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.