



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:48 am BST

PDB ID : 1C3V
Title : DIHYDRODIPICOLINATE REDUCTASE FROM MYCOBACTERIUM TUBERCULOSIS COMPLEXED WITH NADPH AND PDC
Authors : Cirilli, M.; Zheng, R.; Scapin, G.; Blanchard, J.S.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 1999-07-28
Resolution : 2.39 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

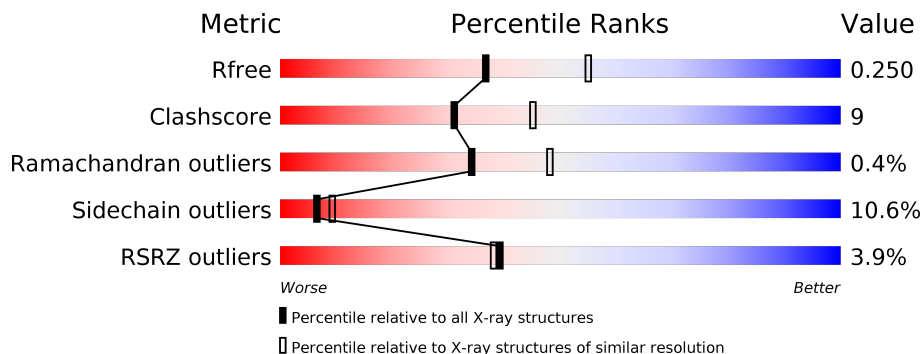
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	245	 4% 73% 24% •
1	B	245	 3% 76% 22% •

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
2	NDP	A	801	X	-	-	-
2	NDP	B	1301	X	-	-	-

2 Entry composition [i](#)

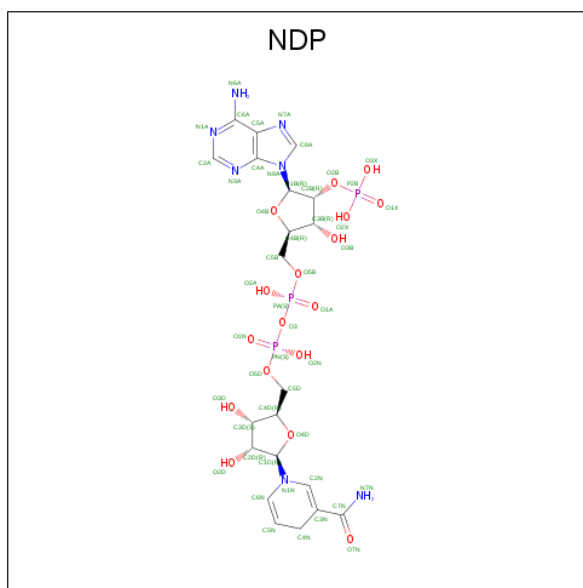
There are 5 unique types of molecules in this entry. The entry contains 3778 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIHYDRODIPICOLINATE REDUCTASE.

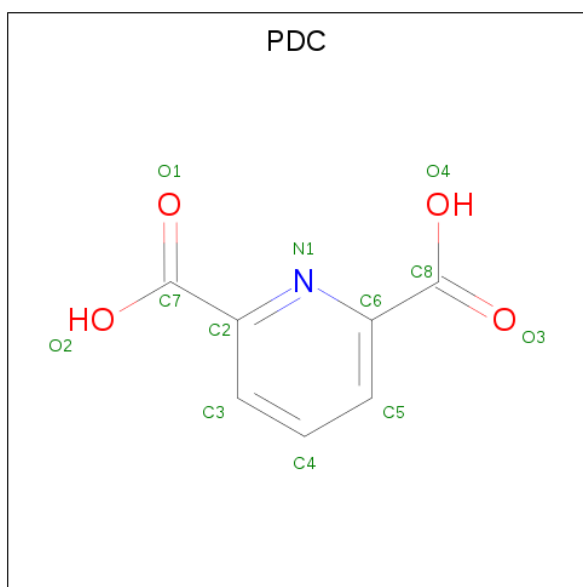
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	245	Total 1808	1141	321	342	4	0	0	0
1	B	245	Total 1812	1144	322	342	4	0	0	0

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



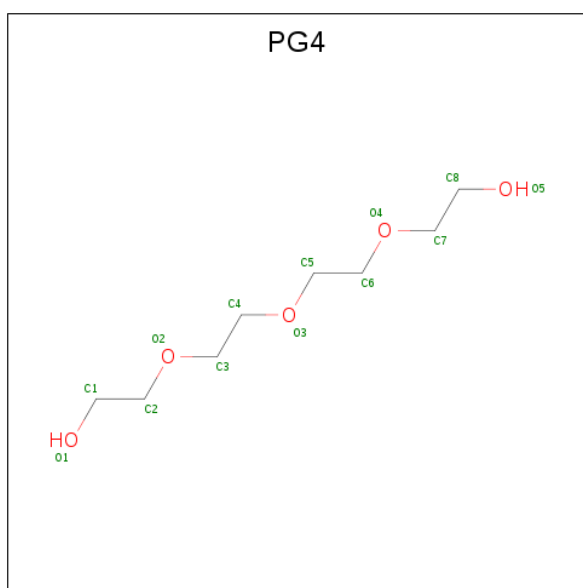
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 48	21	7	17	3	0	0
2	B	1	Total 48	21	7	17	3	0	0

- Molecule 3 is PYRIDINE-2,6-DICARBOXYLIC ACID (three-letter code: PDC) (formula: $C_7H_5NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	12	7	1	4	0	0
3	B	1	12	7	1	4	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	13	8	5	0	0

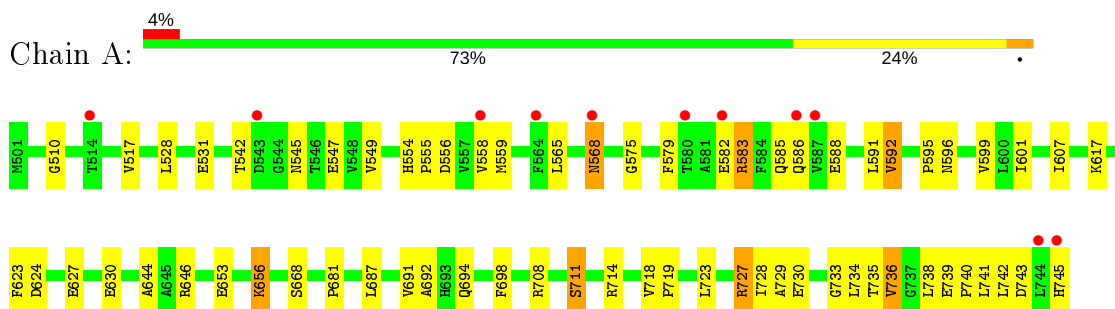
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	8	Total O 8 8	0	0
5	B	17	Total O 17 17	0	0

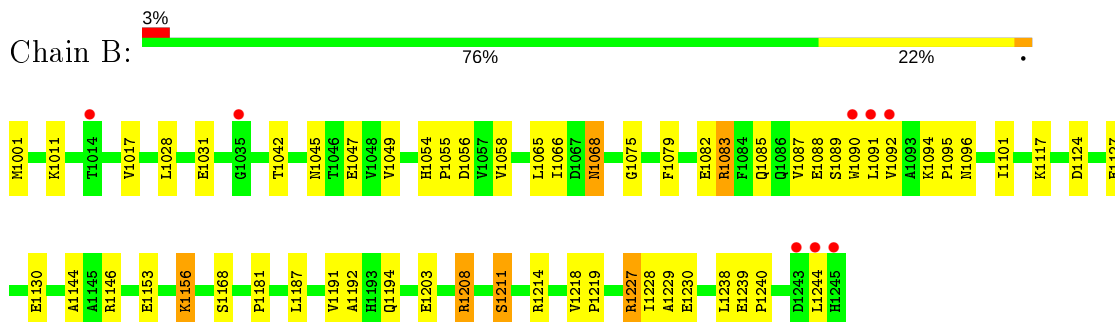
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: DIHYDRODIPICOLINATE REDUCTASE



- Molecule 1: DIHYDRODIPICOLINATE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.83Å 118.26Å 79.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.40 – 2.39 30.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.40-2.39) 79.4 (30.40-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.51Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.193 , 0.243 0.196 , 0.250	Depositor DCC
R_{free} test set	649 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtrriage
Anisotropy	0.146	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.189 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3778	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, PG4, PDC

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	0.33	0/1843	0.86	3/2514 (0.1%)
1	B	0.32	0/1847	0.90	3/2518 (0.1%)
All	All	0.32	0/3690	0.88	6/5032 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1083	ARG	NE-CZ-NH2	-22.34	109.13	120.30
1	B	1083	ARG	NE-CZ-NH1	21.12	130.86	120.30
1	A	583	ARG	NE-CZ-NH1	-20.60	110.00	120.30
1	A	583	ARG	NE-CZ-NH2	19.30	129.95	120.30
1	B	1083	ARG	CD-NE-CZ	14.96	144.54	123.60
1	A	583	ARG	CD-NE-CZ	14.37	143.72	123.60

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	1808	0	1815	36	0
1	B	1812	0	1826	33	0
2	A	48	0	25	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	25	2	0
3	A	12	0	5	0	0
3	B	12	0	5	0	0
4	B	13	0	18	1	0
5	A	8	0	0	0	0
5	B	17	0	0	1	0
All	All	3778	0	3719	68	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 9.

All (68) 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:591:LEU:HD22	1:A:733:GLY:HA2	1.68	0.75
1:A:601:ILE:HD12	1:A:734:LEU:HD11	1.71	0.72
1:B:1011:LYS:HE3	2:B:1301:NDP:O1A	1.93	0.68
1:A:542:THR:HG21	1:A:568:ASN:HD22	1.62	0.64
1:B:1042:THR:HG21	1:B:1068:ASN:HD22	1.63	0.64
1:B:1075:GLY:O	2:B:1301:NDP:H2N	2.00	0.62
1:B:1017:VAL:HG13	1:B:1028:LEU:HD11	1.83	0.61
1:A:517:VAL:HG13	1:A:528:LEU:HD11	1.83	0.61
1:B:1054:HIS:HD2	1:B:1056:ASP:H	1.52	0.58
1:B:1208:ARG:HH22	4:B:2000:PG4:H72	1.69	0.58
1:A:554:HIS:HD2	1:A:556:ASP:H	1.51	0.57
1:A:542:THR:CG2	1:A:568:ASN:HD22	2.18	0.57
1:B:1042:THR:CG2	1:B:1068:ASN:HD22	2.18	0.56
1:B:1028:LEU:HD21	1:B:1031:GLU:HG3	1.88	0.56
1:B:1088:GLU:O	1:B:1092:VAL:HG23	2.06	0.55
1:B:1055:PRO:O	1:B:1083:ARG:NH2	2.39	0.55
1:B:1085:GLN:O	1:B:1088:GLU:HB2	2.08	0.54
1:A:528:LEU:HD21	1:A:531:GLU:HG3	1.88	0.53
1:A:510:GLY:HA3	2:A:801:NDP:H52A	1.89	0.53
1:B:1218:VAL:HB	1:B:1219:PRO:HD3	1.91	0.52
1:B:1066:ILE:HG23	1:B:1091:LEU:HD23	1.90	0.52
1:A:718:VAL:HB	1:A:719:PRO:HD3	1.92	0.52
1:A:579:PHE:CE2	1:A:601:ILE:HD13	2.46	0.51
1:A:601:ILE:O	1:A:736:VAL:HA	2.10	0.50
1:B:1079:PHE:CE2	1:B:1101:ILE:HD13	2.46	0.50
1:A:542:THR:HG21	1:A:568:ASN:ND2	2.27	0.49
1:B:1042:THR:HG21	1:B:1068:ASN:ND2	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:PRO:O	1:A:583:ARG:NH2	2.46	0.48
1:A:691:VAL:HB	1:A:711:SER:O	2.14	0.47
1:B:1153:GLU:HG2	1:B:1156:LYS:NZ	2.29	0.47
1:A:575:GLY:O	2:A:801:NDP:H2N	2.13	0.47
1:A:555:PRO:HA	1:A:558:VAL:HG23	1.96	0.47
1:A:714:ARG:HG3	1:A:714:ARG:HH11	1.80	0.47
1:B:1055:PRO:HA	1:B:1058:VAL:HG23	1.96	0.47
1:B:1214:ARG:HG3	1:B:1214:ARG:HH11	1.80	0.47
1:A:653:GLU:HG2	1:A:656:LYS:NZ	2.30	0.46
1:A:554:HIS:CD2	1:A:556:ASP:H	2.33	0.46
1:B:1191:VAL:HB	1:B:1211:SER:O	2.16	0.46
1:A:559:MET:HG2	1:A:583:ARG:HH21	1.80	0.45
1:A:585:GLN:O	1:A:588:GLU:HB2	2.17	0.45
1:A:592:VAL:O	1:A:595:PRO:HD3	2.18	0.44
1:A:559:MET:HE3	1:A:583:ARG:HB3	1.99	0.44
1:A:728:ILE:HG23	1:A:729:ALA:N	2.33	0.44
1:B:1228:ILE:HG23	1:B:1229:ALA:N	2.33	0.43
1:B:1001:MET:N	5:B:2010:HOH:O	2.51	0.43
1:B:1227:ARG:O	1:B:1230:GLU:HB2	2.18	0.43
1:B:1049:VAL:HG11	1:B:1065:LEU:HD22	2.01	0.43
1:A:727:ARG:O	1:A:730:GLU:HB2	2.19	0.43
1:B:1239:GLU:HB2	1:B:1240:PRO:HD3	1.99	0.43
1:A:723:LEU:HG	1:A:741:LEU:HD23	2.00	0.42
1:A:739:GLU:N	1:A:740:PRO:CD	2.82	0.42
1:A:599:VAL:O	1:A:734:LEU:HA	2.20	0.42
1:B:1192:ALA:HB3	1:B:1211:SER:HB2	2.01	0.42
1:B:1239:GLU:H	1:B:1239:GLU:CD	2.22	0.42
1:A:692:ALA:HB3	1:A:711:SER:HB2	2.01	0.42
1:A:549:VAL:HG11	1:A:565:LEU:HD22	2.01	0.41
1:A:627:GLU:HG2	1:A:681:PRO:HD2	2.02	0.41
1:A:549:VAL:HG11	1:A:565:LEU:CD2	2.50	0.41
1:B:1054:HIS:CD2	1:B:1056:ASP:H	2.33	0.41
1:B:1144:ALA:HA	1:B:1194:GLN:NE2	2.35	0.41
1:B:1049:VAL:HG11	1:B:1065:LEU:CD2	2.50	0.41
1:B:1127:GLU:HG2	1:B:1181:PRO:HD2	2.02	0.41
1:B:1238:LEU:HD12	1:B:1238:LEU:HA	1.96	0.41
1:A:644:ALA:HA	1:A:694:GLN:NE2	2.35	0.41
1:A:623:PHE:CG	1:A:698:PHE:HB3	2.56	0.41
1:A:735:THR:O	1:A:736:VAL:HB	2.21	0.41
1:A:607:ILE:HG22	1:B:1203:GLU:OE2	2.20	0.40
1:B:1083:ARG:O	1:B:1087:VAL:HG23	2.21	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	243/245 (99%)	223 (92%)	19 (8%)	1 (0%)	34	48
1	B	243/245 (99%)	229 (94%)	13 (5%)	1 (0%)	34	48
All	All	486/490 (99%)	452 (93%)	32 (7%)	2 (0%)	34	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	736	VAL
1	B	1095	PRO

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	189/191 (99%)	168 (89%)	21 (11%)	6	8
1	B	190/191 (100%)	171 (90%)	19 (10%)	7	11
All	All	379/382 (99%)	339 (89%)	40 (11%)	6	9

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	545	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	547	GLU
1	A	568	ASN
1	A	582	GLU
1	A	586	GLN
1	A	592	VAL
1	A	596	ASN
1	A	617	LYS
1	A	624	ASP
1	A	630	GLU
1	A	646	ARG
1	A	656	LYS
1	A	668	SER
1	A	687	LEU
1	A	708	ARG
1	A	711	SER
1	A	727	ARG
1	A	738	LEU
1	A	742	LEU
1	A	743	ASP
1	A	745	HIS
1	B	1045	ASN
1	B	1047	GLU
1	B	1068	ASN
1	B	1082	GLU
1	B	1089	SER
1	B	1090	TRP
1	B	1094	LYS
1	B	1096	ASN
1	B	1117	LYS
1	B	1124	ASP
1	B	1130	GLU
1	B	1146	ARG
1	B	1156	LYS
1	B	1168	SER
1	B	1187	LEU
1	B	1208	ARG
1	B	1211	SER
1	B	1227	ARG
1	B	1244	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	554	HIS
1	A	618	GLN
1	A	694	GLN
1	B	1054	HIS
1	B	1086	GLN
1	B	1118	GLN
1	B	1194	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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$
4	PG4	B	2000	-	12,12,12	0.66	0	11,11,11	1.18	0
2	NDP	A	801	-	45,52,52	2.18	8 (17%)	53,80,80	1.98	10 (18%)
3	PDC	B	1302	-	6,12,12	3.57	3 (50%)	8,16,16	1.76	3 (37%)
3	PDC	A	802	-	6,12,12	3.59	3 (50%)	8,16,16	1.86	3 (37%)
2	NDP	B	1301	-	45,52,52	2.15	8 (17%)	53,80,80	1.92	12 (22%)

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
4	PG4	B	2000	-	-	6/10/10/10	-
2	NDP	A	801	-	1/1/14/17	10/30/77/77	0/5/5/5
3	PDC	B	1302	-	-	0/0/8/8	0/1/1/1
3	PDC	A	802	-	-	0/0/8/8	0/1/1/1
2	NDP	B	1301	-	1/1/14/17	14/30/77/77	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	NDP	O7N-C7N	8.29	1.44	1.24
2	A	801	NDP	O7N-C7N	8.11	1.43	1.24
2	A	801	NDP	C4N-C3N	-6.61	1.36	1.49
2	B	1301	NDP	C4N-C3N	-6.40	1.37	1.49
3	B	1302	PDC	C2-N1	6.16	1.44	1.34
3	A	802	PDC	C2-N1	6.09	1.44	1.34
3	A	802	PDC	C6-N1	5.48	1.43	1.34
3	B	1302	PDC	C6-N1	5.22	1.42	1.34
2	A	801	NDP	C7N-C3N	-4.69	1.38	1.48
2	A	801	NDP	C6N-C5N	4.33	1.41	1.33
2	B	1301	NDP	C7N-C3N	-4.32	1.39	1.48
2	B	1301	NDP	C6N-C5N	4.27	1.41	1.33
2	A	801	NDP	C4N-C5N	-3.40	1.40	1.48
2	B	1301	NDP	C4N-C5N	-3.33	1.40	1.48
2	B	1301	NDP	C5A-C4A	-3.13	1.32	1.40
2	A	801	NDP	C5A-C4A	-3.03	1.32	1.40
2	A	801	NDP	C2A-N3A	2.44	1.36	1.32
2	B	1301	NDP	C2A-N3A	2.39	1.35	1.32
2	B	1301	NDP	C3B-C4B	2.39	1.59	1.53
2	A	801	NDP	C3B-C4B	2.35	1.59	1.53
3	B	1302	PDC	C5-C6	2.16	1.43	1.38
3	A	802	PDC	C5-C6	2.15	1.43	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NDP	C1B-N9A-C4A	9.77	143.81	126.64
2	B	1301	NDP	C1B-N9A-C4A	9.22	142.84	126.64
2	B	1301	NDP	O2B-C2B-C1B	4.06	124.71	110.10
2	A	801	NDP	O2B-C2B-C1B	3.91	124.16	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NDP	O5D-C5D-C4D	3.58	121.30	108.99
2	A	801	NDP	O5B-C5B-C4B	3.49	120.99	108.99
2	B	1301	NDP	O5B-C5B-C4B	3.25	120.17	108.99
2	A	801	NDP	C4A-C5A-N7A	3.10	112.63	109.40
2	B	1301	NDP	O5D-C5D-C4D	3.09	119.62	108.99
2	B	1301	NDP	C4A-C5A-N7A	2.93	112.45	109.40
2	A	801	NDP	O3B-C3B-C2B	-2.88	102.98	111.17
2	B	1301	NDP	O3B-C3B-C2B	-2.86	103.05	111.17
3	B	1302	PDC	C5-C6-N1	-2.78	118.36	121.97
3	A	802	PDC	C5-C6-N1	-2.74	118.42	121.97
2	B	1301	NDP	O3B-C3B-C4B	-2.67	103.32	111.05
2	A	801	NDP	O3B-C3B-C4B	-2.63	103.44	111.05
2	A	801	NDP	O2B-C2B-C3B	2.60	121.09	111.68
2	B	1301	NDP	O2B-C2B-C3B	2.53	120.87	111.68
3	A	802	PDC	C5-C6-C8	2.48	123.28	120.19
3	B	1302	PDC	C6-N1-C2	2.29	120.74	118.06
3	A	802	PDC	C6-N1-C2	2.26	120.70	118.06
2	B	1301	NDP	C2A-N1A-C6A	-2.20	115.00	118.75
2	B	1301	NDP	N3A-C2A-N1A	-2.19	125.26	128.68
3	B	1302	PDC	C5-C6-C8	2.12	122.84	120.19
2	B	1301	NDP	O4B-C1B-C2B	2.11	110.25	106.59
2	B	1301	NDP	C3N-C2N-N1N	2.07	126.05	123.10
2	A	801	NDP	C2A-N1A-C6A	-2.03	115.28	118.75
2	A	801	NDP	C3N-C2N-N1N	2.00	125.96	123.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	801	NDP	C1B
2	B	1301	NDP	C1B

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NDP	C5D-O5D-PN-O3
2	A	801	NDP	C5D-O5D-PN-O1N
2	A	801	NDP	C5D-O5D-PN-O2N
2	B	1301	NDP	C5B-O5B-PA-O2A
2	B	1301	NDP	C2B-O2B-P2B-O2X
4	B	2000	PG4	C1-C2-O2-C3
4	B	2000	PG4	O3-C5-C6-O4
2	A	801	NDP	O4D-C4D-C5D-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1301	NDP	O4D-C4D-C5D-O5D
2	A	801	NDP	C3D-C4D-C5D-O5D
2	B	1301	NDP	C3D-C4D-C5D-O5D
2	B	1301	NDP	C2D-C1D-N1N-C2N
2	B	1301	NDP	PN-O3-PA-O5B
4	B	2000	PG4	C8-C7-O4-C6
4	B	2000	PG4	C3-C4-O3-C5
2	A	801	NDP	C2B-O2B-P2B-O3X
2	B	1301	NDP	C5B-O5B-PA-O3
2	B	1301	NDP	C5B-O5B-PA-O1A
2	B	1301	NDP	O4D-C1D-N1N-C2N
2	A	801	NDP	C2D-C1D-N1N-C2N
2	A	801	NDP	O4D-C1D-N1N-C2N
4	B	2000	PG4	C5-C6-O4-C7
2	B	1301	NDP	O4B-C4B-C5B-O5B
2	B	1301	NDP	C2D-C1D-N1N-C6N
2	B	1301	NDP	C3B-C4B-C5B-O5B
2	B	1301	NDP	O4D-C1D-N1N-C6N
2	A	801	NDP	C2D-C1D-N1N-C6N
4	B	2000	PG4	O2-C3-C4-O3
2	A	801	NDP	C2N-C3N-C7N-N7N
2	B	1301	NDP	C2N-C3N-C7N-N7N

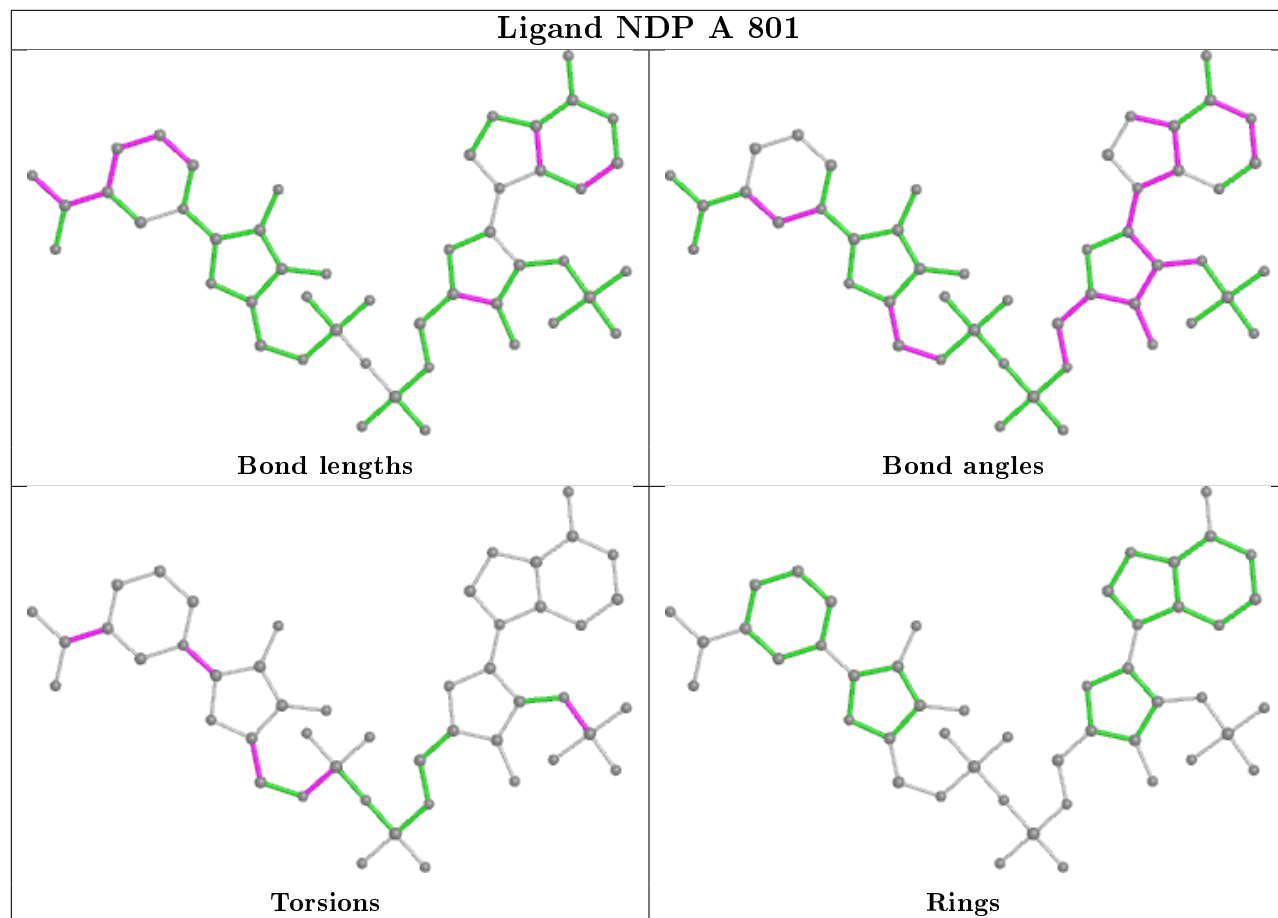
There are no ring outliers.

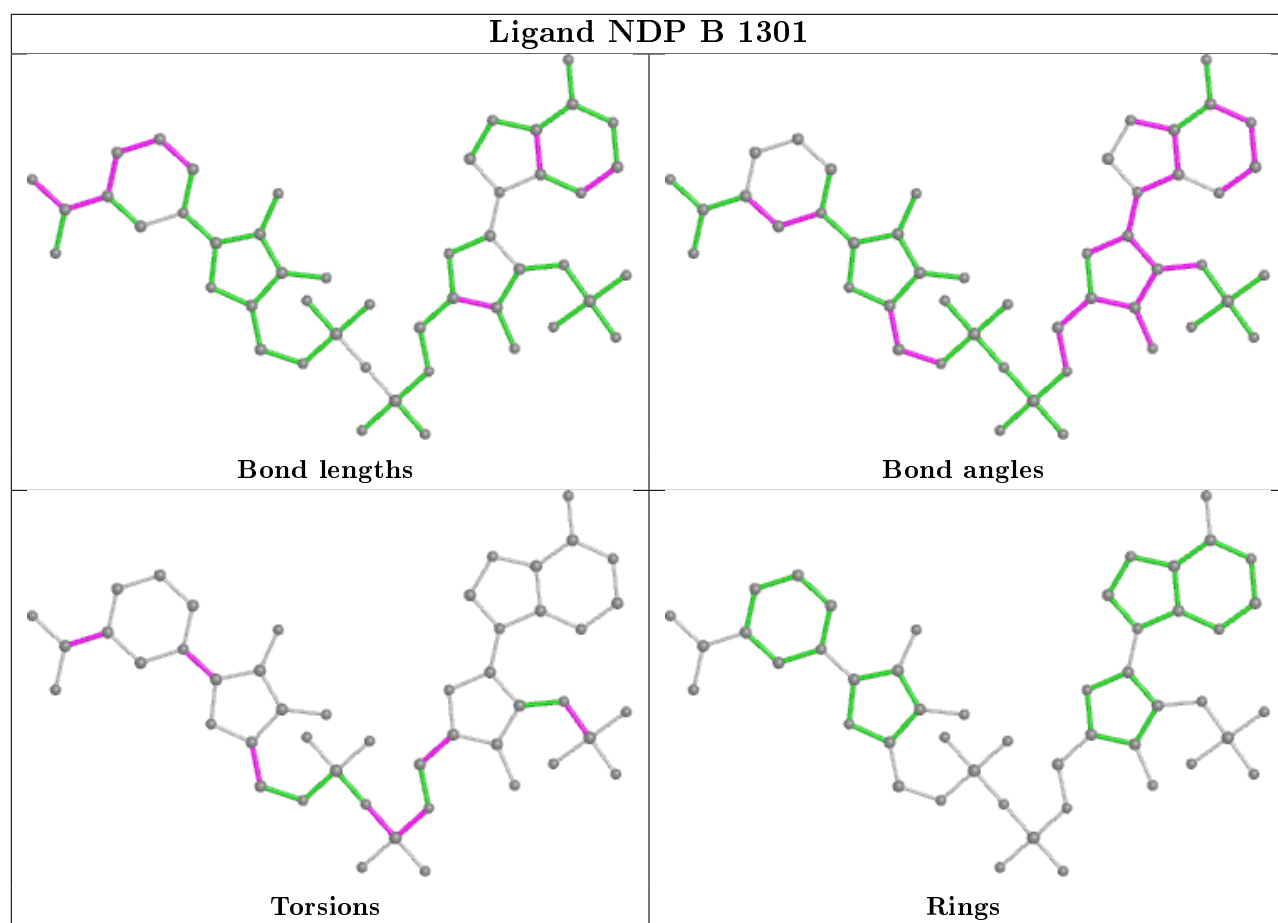
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2000	PG4	1	0
2	A	801	NDP	2	0
2	B	1301	NDP	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	245/245 (100%)	0.21	11 (4%) 33 31	13, 34, 75, 97	0
1	B	245/245 (100%)	0.14	8 (3%) 46 45	13, 34, 75, 98	0
All	All	490/490 (100%)	0.17	19 (3%) 39 38	13, 34, 76, 98	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	745	HIS	8.6
1	B	1245	HIS	4.8
1	A	543	ASP	4.3
1	A	587	VAL	3.7
1	B	1014	THR	3.0
1	B	1035	GLY	2.9
1	B	1244	LEU	2.7
1	B	1090	TRP	2.6
1	A	586	GLN	2.4
1	B	1243	ASP	2.3
1	A	744	LEU	2.3
1	B	1092	VAL	2.2
1	A	514	THR	2.2
1	A	564	PHE	2.2
1	A	558	VAL	2.1
1	B	1091	LEU	2.1
1	A	568	ASN	2.1
1	A	582	GLU	2.1
1	A	580	THR	2.1

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](#)

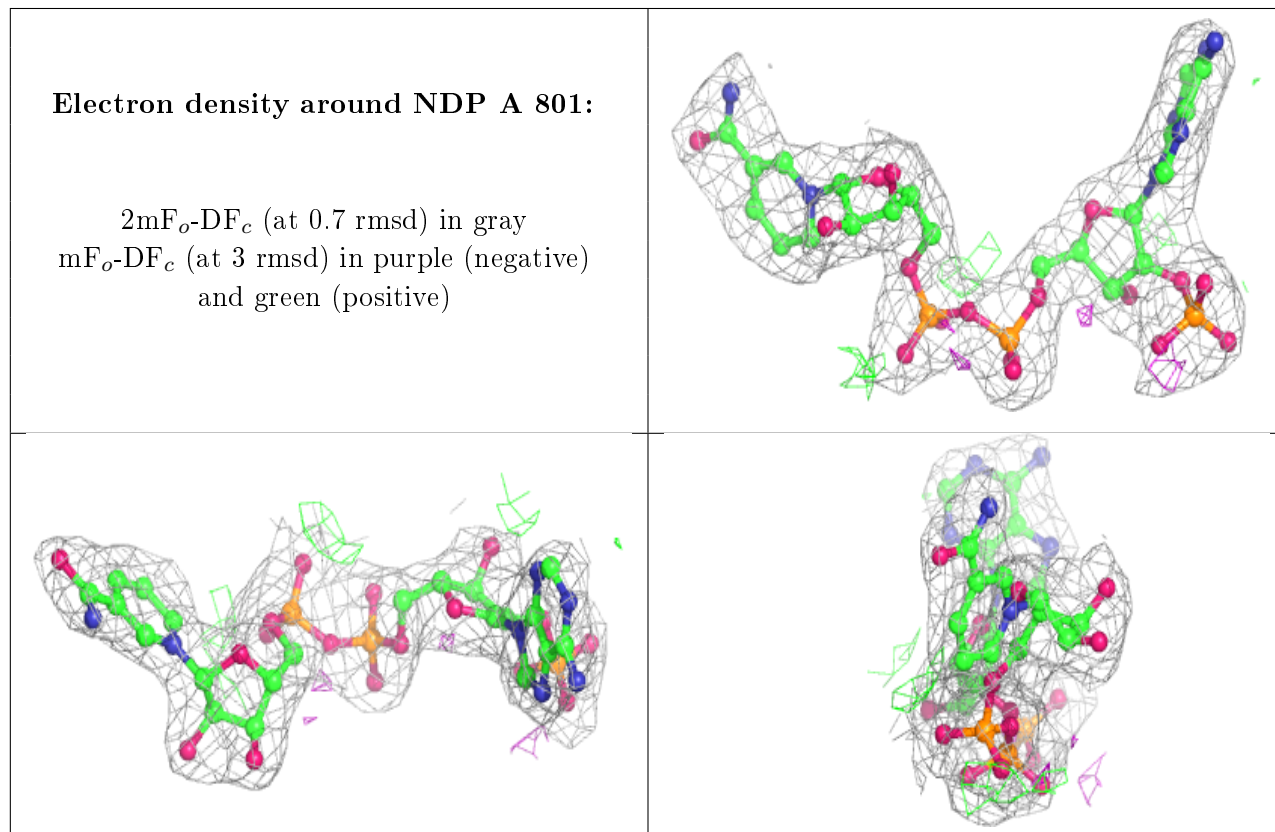
There are no carbohydrates in this entry.

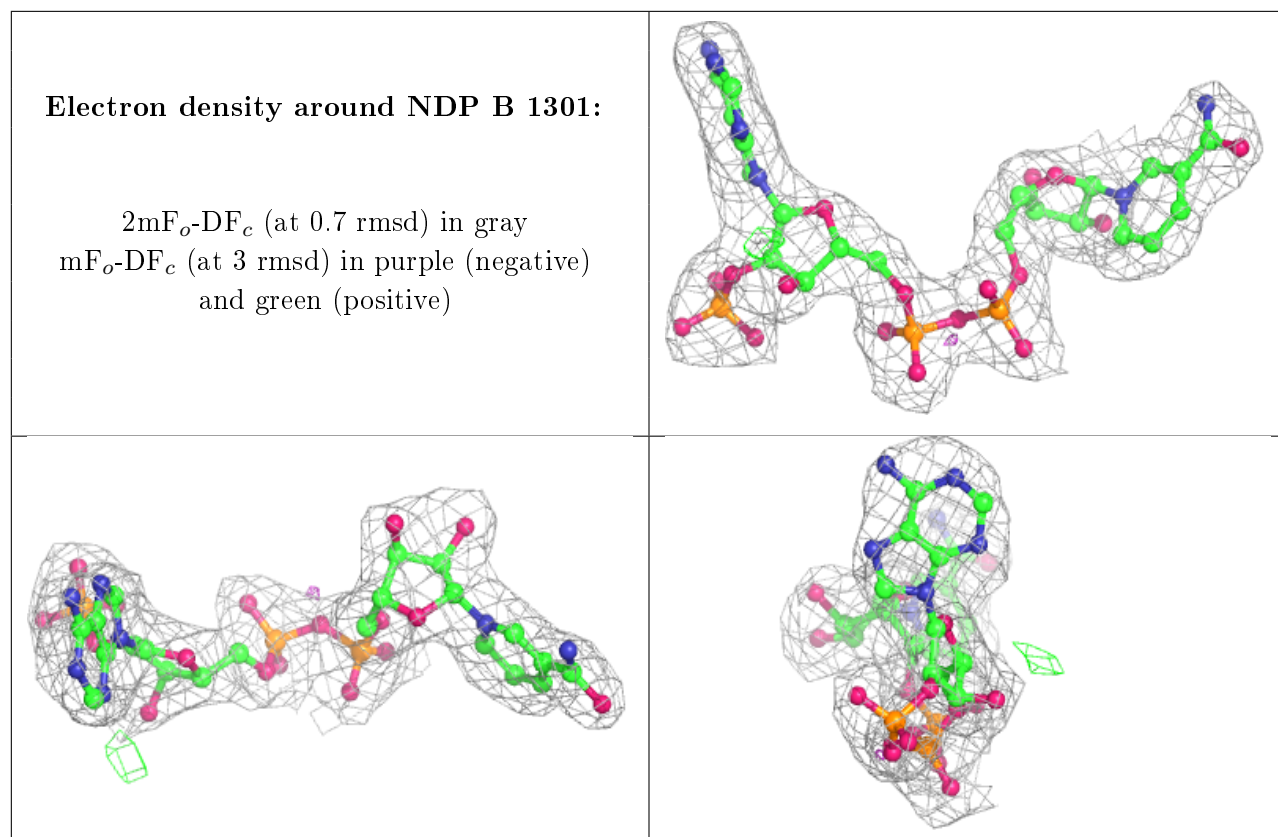
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
4	PG4	B	2000	13/13	0.92	0.15	24,28,29,32	0
2	NDP	A	801	48/48	0.94	0.13	25,45,63,63	0
2	NDP	B	1301	48/48	0.95	0.12	27,37,59,61	0
3	PDC	A	802	12/12	0.96	0.13	15,18,24,26	0
3	PDC	B	1302	12/12	0.96	0.12	15,19,20,23	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.