



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:53 pm BST

PDB ID : 3D3F
Title : Crystal Structure of Yvgn and cofactor NADPH from Bacillus subtilis
Authors : Zhou, Y.F.; Lei, J.; Su, X.D.
Deposited on : 2008-05-10
Resolution : 2.40 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

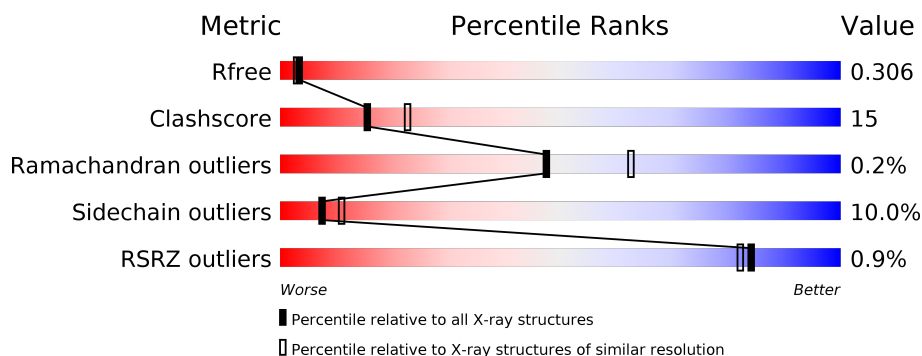
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	275	<div> <div></div> <div> <div></div> <div>67%</div> <div>27%</div> <div>6%</div> </div> </div>
1	B	275	<div> <div></div> <div> <div></div> <div>72%</div> <div>23%</div> <div>5%</div> </div> </div>

2 Entry composition [i](#)

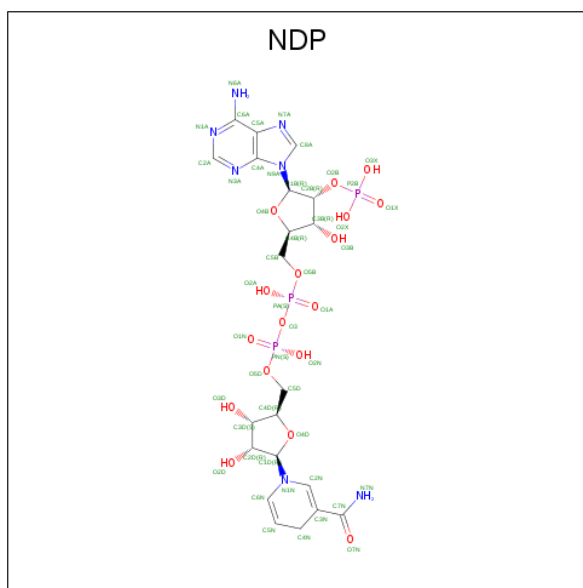
There are 3 unique types of molecules in this entry. The entry contains 4629 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 YvgN protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	1	0
			2226	1417	378	426	5			
1	B	275	Total	C	N	O	S	0	1	0
			2226	1417	378	426	5			

- 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
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		

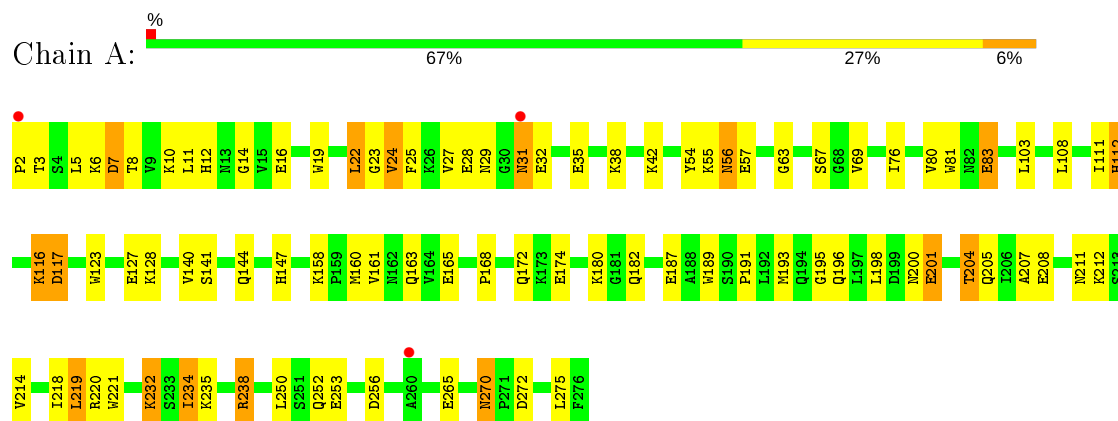
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total 41	O 41	0	0
3	B	40	Total 40	O 40	0	0

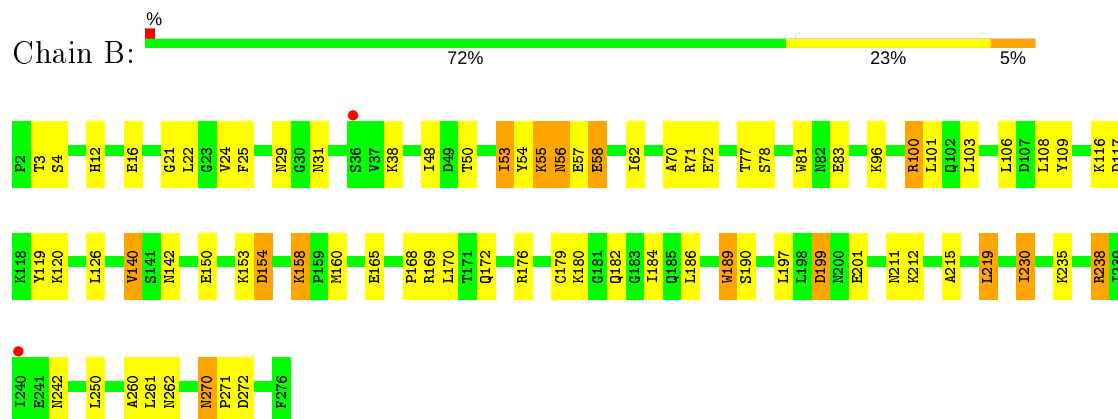
3 Residue-property plots [i](#)

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: YvgN protein



• Molecule 1: YvgN protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	80.52Å 123.28Å 57.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 67.41 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.8 (20.00-2.40) 89.5 (67.41-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.306 0.242 , 0.306	Depositor DCC
R_{free} test set	1156 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.695	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 28.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4629	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2898e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	1.08	5/2271 (0.2%)	0.98	6/3065 (0.2%)
1	B	1.00	2/2271 (0.1%)	0.95	5/3065 (0.2%)
All	All	1.04	7/4542 (0.2%)	0.97	11/6130 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	VAL	CB-CG1	-8.52	1.34	1.52
1	A	117	ASP	CB-CG	-8.06	1.34	1.51
1	A	57	GLU	CD-OE2	-6.96	1.18	1.25
1	A	57	GLU	CD-OE1	-6.44	1.18	1.25
1	A	24	VAL	CB-CG2	-5.49	1.41	1.52
1	B	189	TRP	CE3-CZ3	-5.14	1.29	1.38
1	B	16	GLU	CG-CD	-5.07	1.44	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	LYS	CB-CA-C	-7.24	95.92	110.40
1	A	116	LYS	N-CA-C	7.06	130.07	111.00
1	A	7	ASP	CB-CA-C	-5.85	98.69	110.40
1	B	260	ALA	CB-CA-C	5.55	118.43	110.10
1	A	29	ASN	CB-CA-C	5.24	120.88	110.40
1	B	219	LEU	CB-CG-CD1	5.16	119.77	111.00
1	A	22	LEU	CA-CB-CG	5.15	127.15	115.30
1	B	140	VAL	CG1-CB-CG2	5.13	119.12	110.90
1	A	220	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	A	22	LEU	CB-CG-CD2	5.05	119.59	111.00
1	B	116	LYS	C-N-CA	-5.05	109.08	121.70

There are no chirality outliers.

There are no planarity outliers.

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	2226	0	2210	80	0
1	B	2226	0	2209	65	0
2	A	48	0	26	2	0
2	B	48	0	26	8	0
3	A	41	0	0	4	0
3	B	40	0	0	1	0
All	All	4629	0	4471	133	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.

All (133) 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:55:LYS:HG2	1:B:55:LYS:CG	1.76	1.15
1:A:8:THR:HG21	1:A:16:GLU:HB3	1.29	1.14
1:A:55:LYS:CG	1:B:55:LYS:HG2	1.81	1.09
1:A:8:THR:CG2	1:A:16:GLU:HB3	1.92	0.98
1:A:144:GLN:H	1:A:147:HIS:HD2	1.14	0.94
1:A:27:VAL:CG2	1:A:234:ILE:HD11	2.03	0.88
1:A:27:VAL:HG22	1:A:234:ILE:CD1	2.04	0.87
1:B:242:ASN:HD21	2:B:1:NDP:H2A	1.38	0.86
1:B:190:SER:HA	2:B:1:NDP:O1N	1.76	0.84
1:A:28:GLU:HG3	1:B:96:LYS:NZ	1.94	0.82
1:A:27:VAL:CG2	1:A:234:ILE:CD1	2.59	0.80
1:A:8:THR:HG21	1:A:16:GLU:CB	2.11	0.80
1:A:144:GLN:H	1:A:147:HIS:CD2	2.01	0.79
1:A:55:LYS:CE	1:B:55:LYS:HD3	2.12	0.78
1:A:200:ASN:O	1:A:204:THR:HG23	1.85	0.77
1:B:54:TYR:OH	2:B:1:NDP:H2D	1.85	0.77
1:B:158:LYS:HE3	1:B:182:GLN:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLY:HA3	3:A:296:HOH:O	1.88	0.72
1:B:270:ASN:ND2	1:B:272:ASP:H	1.88	0.71
1:A:55:LYS:HG2	1:B:55:LYS:HG2	0.84	0.71
1:A:28:GLU:HG3	1:B:96:LYS:HZ3	1.53	0.70
1:A:27:VAL:HG22	1:A:234:ILE:HD11	1.69	0.70
1:A:55:LYS:HE3	1:B:55:LYS:HD3	1.73	0.70
1:A:270:ASN:HD22	1:A:272:ASP:H	1.41	0.69
1:A:27:VAL:HG22	1:A:234:ILE:HD13	1.75	0.69
1:B:242:ASN:ND2	2:B:1:NDP:H2A	2.07	0.68
1:B:56:ASN:H	1:B:56:ASN:ND2	1.92	0.68
1:A:28:GLU:CG	1:B:96:LYS:NZ	2.58	0.67
1:B:53:ILE:HG12	1:B:81:TRP:CD2	2.33	0.64
1:A:27:VAL:HG21	1:A:234:ILE:HD11	1.78	0.64
1:B:120:LYS:NZ	1:B:154:ASP:HB2	2.13	0.64
1:B:158:LYS:CE	1:B:182:GLN:O	2.46	0.64
1:A:144:GLN:N	1:A:147:HIS:HD2	1.93	0.62
1:A:165:GLU:O	1:A:172:GLN:NE2	2.28	0.62
1:A:54:TYR:O	1:A:55:LYS:HB2	1.99	0.62
1:B:190:SER:CA	2:B:1:NDP:O1N	2.48	0.62
1:B:56:ASN:HD22	1:B:56:ASN:H	1.49	0.61
1:B:270:ASN:HD22	1:B:271:PRO:N	1.99	0.61
1:A:270:ASN:ND2	1:A:272:ASP:HB2	2.17	0.59
1:A:116:LYS:HD2	1:A:275:LEU:HB3	1.84	0.59
1:B:211:ASN:O	1:B:212:LYS:HD3	2.02	0.59
1:A:3:THR:N	1:A:7:ASP:OD2	2.36	0.59
1:A:8:THR:CG2	1:A:16:GLU:CB	2.75	0.58
1:A:12:HIS:CE1	1:A:160:MET:HG3	2.39	0.57
1:A:27:VAL:HG21	1:A:234:ILE:CD1	2.34	0.57
1:B:142:ASN:O	1:B:271:PRO:HB3	2.04	0.57
1:A:28:GLU:CG	1:B:96:LYS:HZ2	2.17	0.57
1:B:172:GLN:O	1:B:176:ARG:HG3	2.04	0.57
1:B:12:HIS:CE1	1:B:160:MET:HG2	2.40	0.57
1:B:168:PRO:O	1:B:262:ASN:HA	2.05	0.56
1:A:56:ASN:HD22	1:A:56:ASN:C	2.08	0.56
1:A:207:ALA:HB1	1:A:212:LYS:O	2.06	0.56
1:A:27:VAL:CG2	1:A:234:ILE:HD13	2.34	0.56
1:B:270:ASN:HD22	1:B:272:ASP:H	1.54	0.55
1:A:198:LEU:HA	1:A:214:VAL:HG11	1.88	0.55
1:A:55:LYS:CD	1:B:55:LYS:HD3	2.36	0.55
1:B:57:GLU:OE1	1:B:100:ARG:NH1	2.39	0.55
1:A:270:ASN:HD21	1:A:272:ASP:HB2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:GLU:HB2	1:B:189:TRP:CZ2	2.42	0.55
1:B:53:ILE:HG12	1:B:81:TRP:CG	2.42	0.54
1:A:232:LYS:O	2:A:1:NDP:H8A	2.08	0.54
1:B:58:GLU:O	1:B:62:ILE:HG13	2.08	0.53
1:A:111:ILE:O	1:A:141:SER:HB3	2.09	0.53
1:B:165:GLU:HB2	1:B:189:TRP:CH2	2.44	0.53
1:B:50:THR:O	1:B:78:SER:HA	2.09	0.53
1:B:29:ASN:HD21	1:B:58:GLU:HG3	1.75	0.52
1:A:25:PHE:CZ	1:B:83:GLU:HG3	2.45	0.52
1:B:189:TRP:CD2	2:B:1:NDP:H41N	2.44	0.52
1:A:8:THR:HG23	1:A:16:GLU:HB3	1.86	0.52
1:B:165:GLU:O	1:B:172:GLN:NE2	2.38	0.52
1:A:158:LYS:HD3	1:A:182:GLN:O	2.10	0.51
1:A:117:ASP:O	3:A:277:HOH:O	2.19	0.51
2:B:1:NDP:H3D	2:B:1:NDP:H6N	1.93	0.51
1:A:235:LYS:HB2	1:A:238:ARG:HG3	1.94	0.50
1:B:96:LYS:O	1:B:100:ARG:HG2	2.11	0.50
1:A:76:ILE:HG21	1:A:103:LEU:HD11	1.94	0.50
1:A:11:LEU:HD13	1:A:160:MET:HB3	1.94	0.49
1:A:193:MET:CE	1:A:196:GLN:HB2	2.41	0.49
1:B:215:ALA:O	1:B:219:LEU:HG	2.13	0.49
1:A:32:GLU:HG2	1:A:234:ILE:HG13	1.94	0.48
1:A:81:TRP:CD1	1:A:83:GLU:HB3	2.49	0.48
1:B:21:GLY:HA3	1:B:230:ILE:HG22	1.96	0.48
1:B:270:ASN:HD22	1:B:271:PRO:CD	2.27	0.48
1:A:218:ILE:O	1:A:221:TRP:HB3	2.14	0.47
1:A:200:ASN:O	1:A:204:THR:CG2	2.61	0.47
1:B:270:ASN:HD22	1:B:270:ASN:C	2.18	0.47
1:A:211:ASN:O	1:A:212:LYS:HD3	2.15	0.46
1:A:270:ASN:ND2	1:A:272:ASP:H	2.12	0.46
1:A:201:GLU:H	1:A:201:GLU:HG2	1.60	0.46
1:B:25:PHE:HB2	2:B:1:NDP:H2D	1.98	0.46
1:B:109:TYR:HD2	1:B:126:LEU:HD22	1.81	0.46
1:A:163:GLN:NE2	1:A:187:GLU:OE2	2.47	0.45
1:A:27:VAL:HG23	1:A:232:LYS:HE2	1.98	0.45
1:B:120:LYS:HZ1	1:B:154:ASP:HB2	1.80	0.45
1:A:158:LYS:HB3	3:A:308:HOH:O	2.16	0.44
1:B:56:ASN:N	1:B:56:ASN:HD22	2.11	0.44
1:B:197:LEU:C	1:B:199:ASP:H	2.19	0.44
1:B:169:ARG:HG2	1:B:197:LEU:HD21	1.98	0.44
1:B:77:THR:HA	1:B:108:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HB3	1:B:48:ILE:HD13	1.98	0.44
1:B:71:ARG:HD2	1:B:71:ARG:HA	1.85	0.44
1:A:2:PRO:HG3	1:A:19:TRP:CD1	2.54	0.43
1:B:4:SER:HA	3:B:315:HOH:O	2.17	0.43
1:A:55:LYS:HE3	1:B:55:LYS:CD	2.46	0.43
1:B:56:ASN:N	1:B:56:ASN:ND2	2.54	0.43
1:B:179:CYS:HB3	1:B:184:ILE:O	2.17	0.43
1:A:165:GLU:HB2	1:A:189:TRP:CH2	2.53	0.43
1:B:101:LEU:HB3	1:B:103:LEU:HG	1.99	0.43
1:A:35:GLU:OE2	1:A:38:LYS:HE2	2.17	0.43
1:B:70:ALA:O	1:B:71:ARG:C	2.58	0.43
1:A:63:GLY:O	1:A:67:SER:HB3	2.19	0.42
1:A:24:VAL:O	1:A:27:VAL:HB	2.19	0.42
1:A:198:LEU:HB3	3:A:302:HOH:O	2.19	0.42
1:A:123:TRP:O	1:A:127:GLU:HG3	2.19	0.42
1:A:193:MET:HE2	1:A:196:GLN:HB2	2.02	0.42
1:B:81:TRP:HD1	1:B:83:GLU:HB3	1.85	0.42
1:A:31:ASN:HA	1:A:31:ASN:HD22	1.57	0.42
1:B:165:GLU:O	1:B:170:LEU:HD23	2.20	0.42
1:A:108:LEU:HD21	1:A:161:VAL:HG21	2.02	0.41
1:A:204:THR:O	1:A:208:GLU:HG3	2.20	0.41
1:B:106:LEU:HD12	1:B:109:TYR:CD1	2.55	0.41
1:A:28:GLU:HG2	1:B:96:LYS:HZ2	1.85	0.41
1:A:219:LEU:HA	1:A:219:LEU:HD12	1.98	0.41
1:A:193:MET:HE3	1:A:196:GLN:HB2	2.02	0.41
1:A:252:GLN:NE2	1:A:256:ASP:OD1	2.53	0.41
1:A:10:LYS:HG2	1:A:14:GLY:HA2	2.02	0.41
1:A:189:TRP:CD2	2:A:1:NDP:H41N	2.56	0.41
1:B:119:TYR:OH	1:B:150:GLU:HG2	2.21	0.40
1:A:23:GLY:O	1:A:232:LYS:HB2	2.20	0.40
1:A:27:VAL:CG1	1:A:234:ILE:HD11	2.52	0.40
1:B:235:LYS:HD2	1:B:238:ARG:HE	1.86	0.40
1:A:80:VAL:O	1:A:112:HIS:HB2	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	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
1	B	273/275 (99%)	248 (91%)	24 (9%)	1 (0%)	34	48
All	All	546/550 (99%)	512 (94%)	33 (6%)	1 (0%)	47	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	261	LEU

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	241/241 (100%)	216 (90%)	25 (10%)	7	10
1	B	241/241 (100%)	218 (90%)	23 (10%)	8	12
All	All	482/482 (100%)	434 (90%)	48 (10%)	7	11

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	LYS
1	A	22	LEU
1	A	31	ASN
1	A	42	LYS

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Mol	Chain	Res	Type
1	A	56	ASN
1	A	69	VAL
1	A	83	GLU
1	A	112	HIS
1	A	128	LYS
1	A	140	VAL
1	A	168	PRO
1	A	174	GLU
1	A	180	LYS
1	A	201	GLU
1	A	204	THR
1	A	205	GLN
1	A	219	LEU
1	A	232	LYS
1	A	234	ILE
1	A	238	ARG
1	A	250	LEU
1	A	253	GLU
1	A	265	GLU
1	A	270	ASN
1	B	3	THR
1	B	24	VAL
1	B	31	ASN
1	B	38	LYS
1	B	53	ILE
1	B	55	LYS
1	B	56	ASN
1	B	58	GLU
1	B	72	GLU
1	B	100	ARG
1	B	117	ASP
1	B	140	VAL
1	B	153	LYS
1	B	154	ASP
1	B	158	LYS
1	B	180	LYS
1	B	186	LEU
1	B	199	ASP
1	B	201	GLU
1	B	230	ILE
1	B	238	ARG
1	B	250	LEU

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Mol	Chain	Res	Type
1	B	270	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	31	ASN
1	A	56	ASN
1	A	147	HIS
1	A	162	ASN
1	A	252	GLN
1	A	270	ASN
1	B	12	HIS
1	B	56	ASN
1	B	162	ASN
1	B	185	GLN
1	B	211	ASN
1	B	270	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	B	1	-	45,52,52	1.58	4 (8%)	53,80,80	1.64	11 (20%)
2	NDP	A	1	-	45,52,52	1.55	5 (11%)	53,80,80	1.38	4 (7%)

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	B	1	-	-	11/30/77/77	0/5/5/5
2	NDP	A	1	-	-	8/30/77/77	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NDP	O7N-C7N	6.47	1.39	1.24
2	B	1	NDP	O7N-C7N	6.17	1.39	1.24
2	B	1	NDP	C2A-N3A	5.32	1.40	1.32
2	A	1	NDP	C2A-N3A	4.32	1.39	1.32
2	B	1	NDP	C2A-N1A	3.54	1.40	1.33
2	A	1	NDP	C6N-C5N	2.91	1.38	1.33
2	A	1	NDP	C2A-N1A	2.87	1.39	1.33
2	A	1	NDP	O4B-C1B	2.34	1.44	1.41
2	B	1	NDP	C6N-C5N	2.13	1.37	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	NDP	N3A-C2A-N1A	-5.48	120.12	128.68
2	B	1	NDP	C3B-C2B-C1B	-4.22	94.95	102.89
2	B	1	NDP	C1B-N9A-C4A	3.77	133.26	126.64
2	B	1	NDP	N3A-C2A-N1A	-3.76	122.80	128.68
2	A	1	NDP	C1D-N1N-C2N	-3.68	114.98	121.11
2	B	1	NDP	C5A-C6A-N6A	-3.46	115.10	120.35
2	B	1	NDP	O7N-C7N-C3N	-3.32	114.65	120.90
2	B	1	NDP	O5D-PN-O1N	-3.06	97.11	109.07
2	B	1	NDP	N6A-C6A-N1A	2.87	124.53	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NDP	C3N-C7N-N7N	2.80	122.63	117.67
2	B	1	NDP	O3D-C3D-C2D	2.33	119.36	111.82
2	B	1	NDP	C1D-N1N-C2N	-2.24	117.39	121.11
2	A	1	NDP	O7N-C7N-C3N	-2.13	116.89	120.90
2	A	1	NDP	C2D-C1D-N1N	-2.10	108.03	113.30
2	B	1	NDP	O3B-C3B-C4B	-2.08	105.05	111.05

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NDP	C5B-O5B-PA-O1A
2	B	1	NDP	C5B-O5B-PA-O3
2	B	1	NDP	C5D-O5D-PN-O1N
2	B	1	NDP	O4D-C4D-C5D-O5D
2	A	1	NDP	C5D-O5D-PN-O2N
2	B	1	NDP	C3D-C4D-C5D-O5D
2	A	1	NDP	O4D-C1D-N1N-C2N
2	A	1	NDP	PA-O3-PN-O1N
2	B	1	NDP	O4D-C1D-N1N-C2N
2	B	1	NDP	C2B-O2B-P2B-O3X
2	B	1	NDP	C5D-O5D-PN-O3
2	A	1	NDP	C5D-O5D-PN-O3
2	B	1	NDP	C5B-O5B-PA-O2A
2	B	1	NDP	C5D-O5D-PN-O2N
2	A	1	NDP	C5D-O5D-PN-O1N
2	A	1	NDP	C4D-C5D-O5D-PN
2	A	1	NDP	PA-O3-PN-O5D
2	B	1	NDP	C2B-O2B-P2B-O2X
2	A	1	NDP	C5B-O5B-PA-O1A

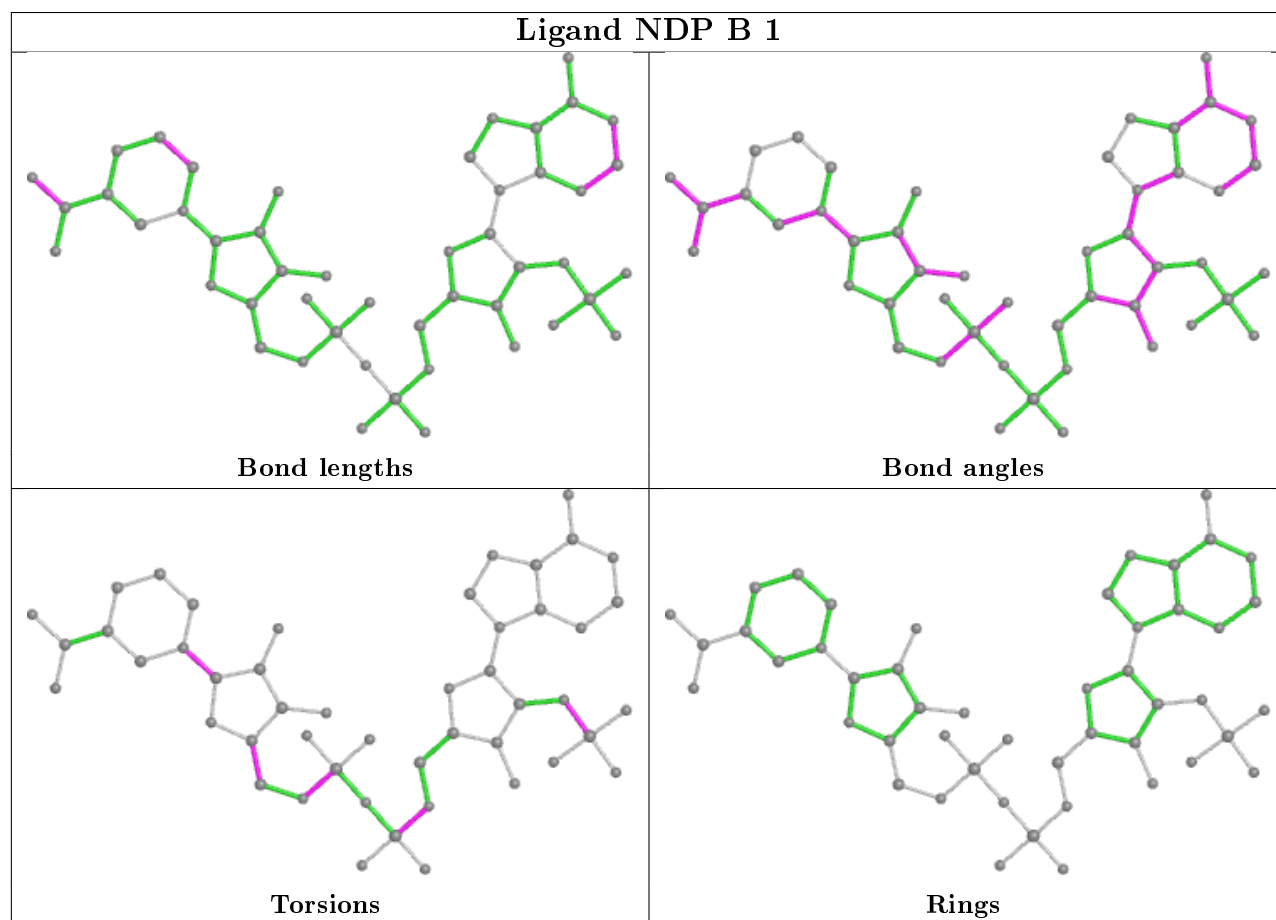
There are no ring outliers.

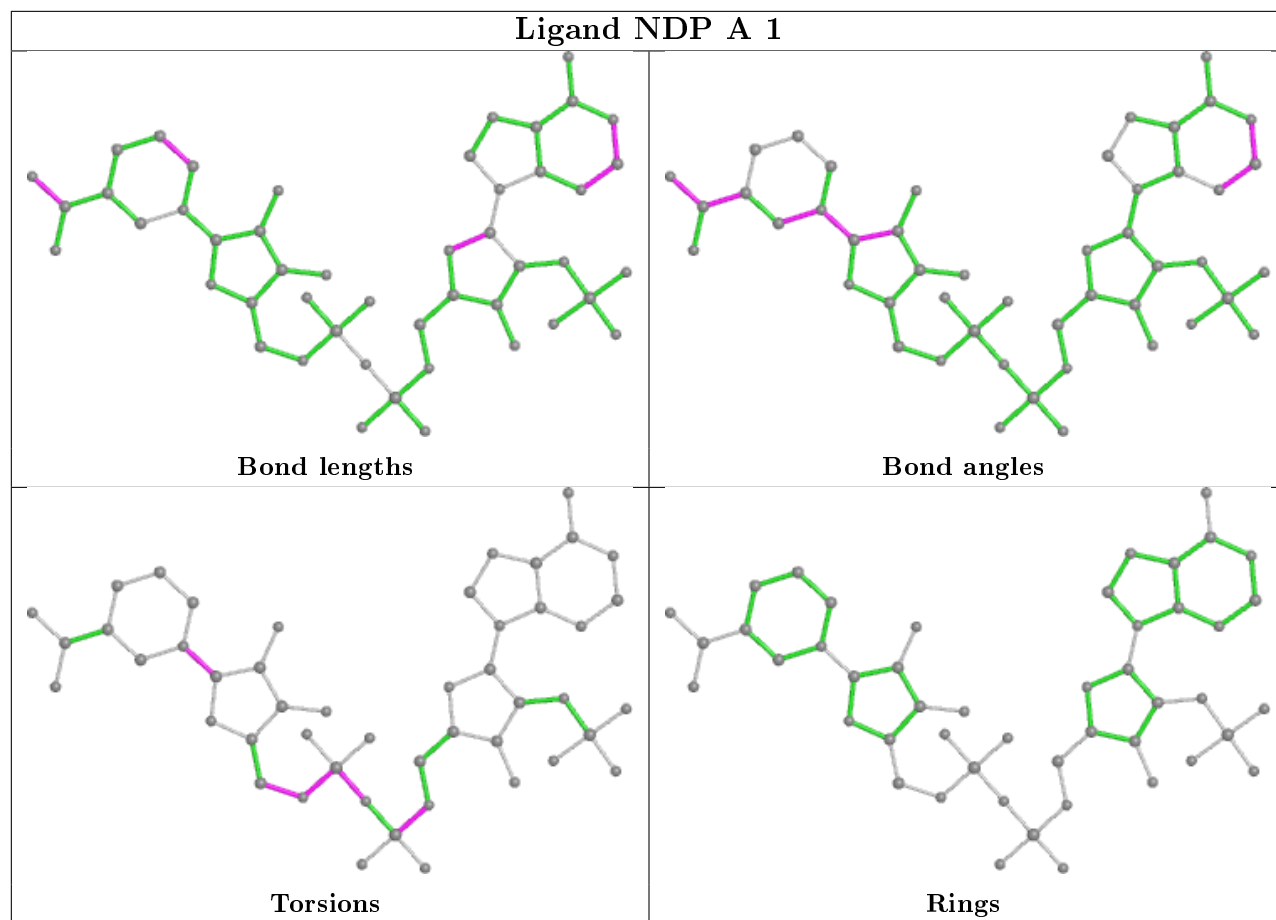
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NDP	8	0
2	A	1	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	275/275 (100%)	-0.15	3 (1%) 80 79	4, 9, 16, 24	1 (0%)
1	B	275/275 (100%)	-0.07	2 (0%) 87 86	2, 9, 16, 22	1 (0%)
All	All	550/550 (100%)	-0.11	5 (0%) 84 82	2, 9, 16, 24	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36[A]	SER	3.6
1	A	260	ALA	3.5
1	A	2	PRO	3.0
1	B	240	ILE	2.7
1	A	31	ASN	2.4

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](#)

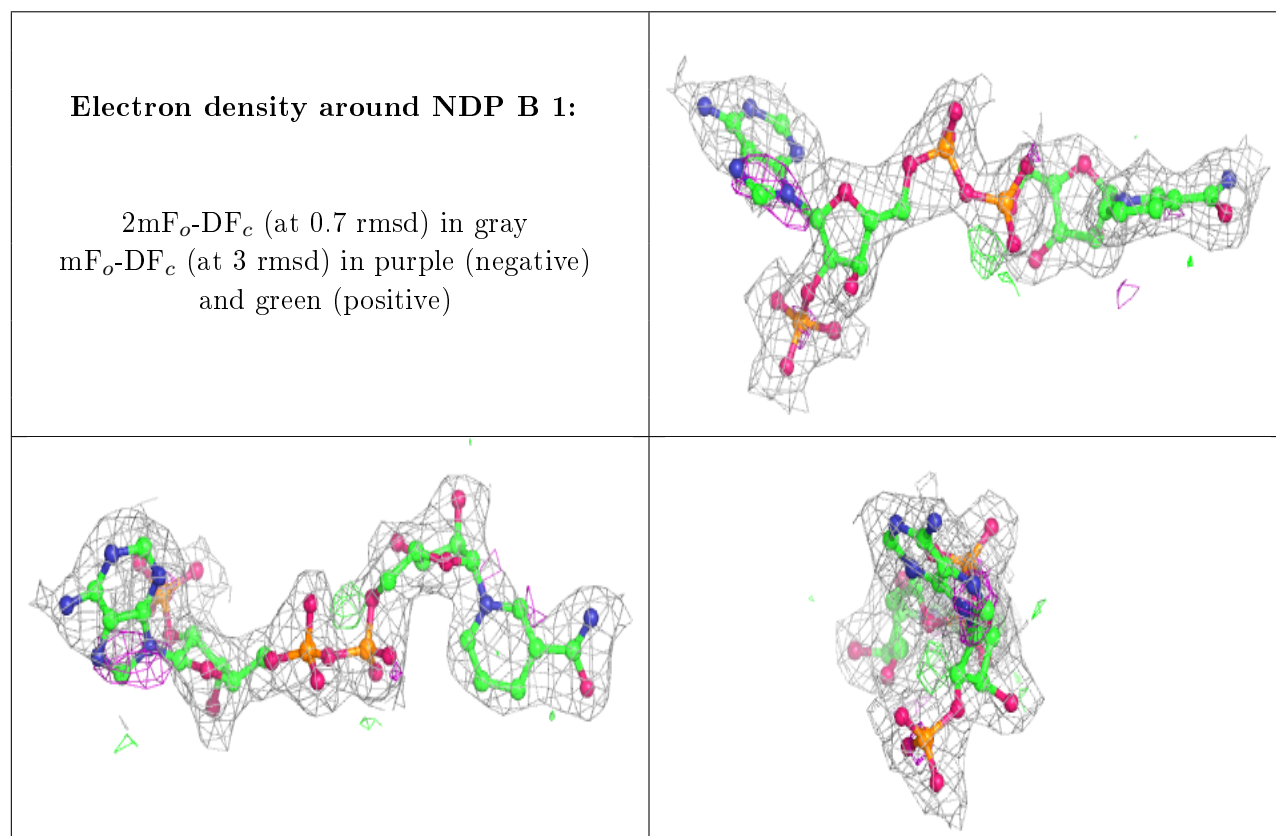
There are no carbohydrates in this entry.

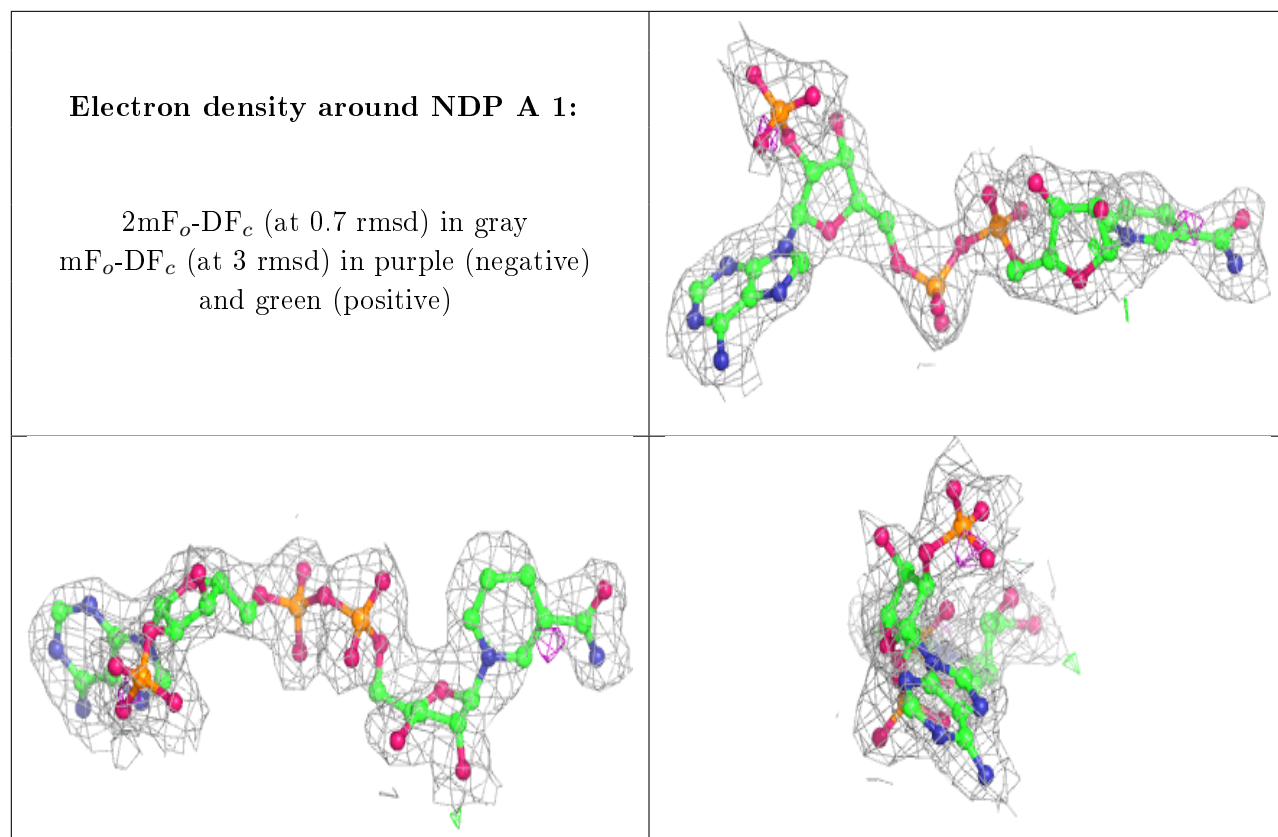
6.4 Ligands [i](#)

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
2	NDP	B	1	48/48	0.91	0.15	5,11,16,19	0
2	NDP	A	1	48/48	0.94	0.15	2,12,16,18	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.