WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 06:04 PM JST

PDB ID	:	7DN1
Title	:	Hetero-oligomers of SCR-SCR2 crystal structure with NADPH
Authors	:	Li, Y.H.; Zhang, R.Z.; Forouhar, F.; Wang, C.; Montelione, G.T.; Szyperski, T.; Xu, Y.; Hunt, J.F.
Deposited on	:	2020-12-08
Resolution	:	1.74 Å(reported)

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

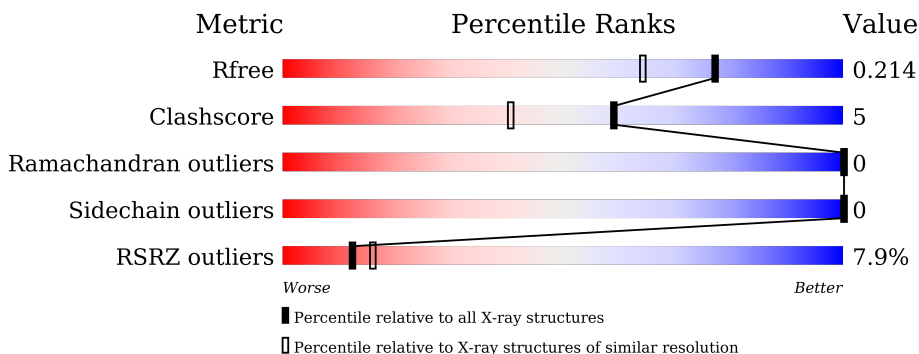|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.74 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.214
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		7.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

⫾ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	280	8% / 90% / 9% ·
2	B	280	8% / 90% / 10%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4581 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 Carbonyl Reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total 2127	C 1353	N 348	O 419	S 7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP B2KJ46

- Molecule 2 is a protein called (S)-specific carbonyl reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	280	Total 2115	C 1343	N 349	O 414	S 9	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP D5G304

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

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total	O	0	0
			124	124		
4	B	119	Total	O	0	0
			119	119		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Carbonyl Reductase
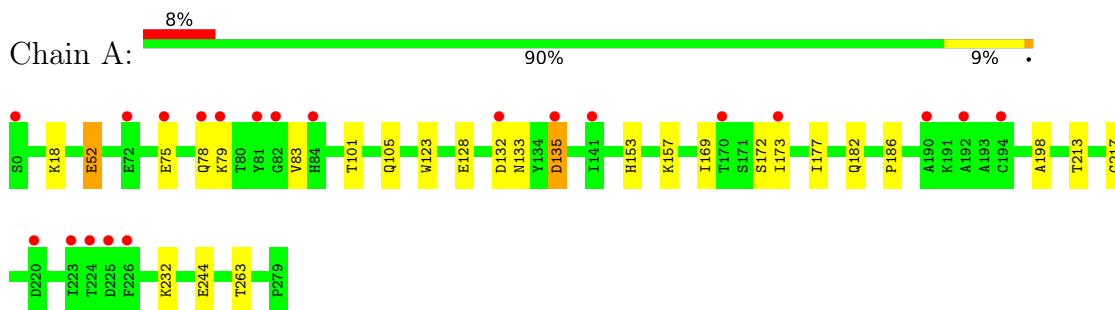
- Molecule 2: (S)-specific carbonyl reductase
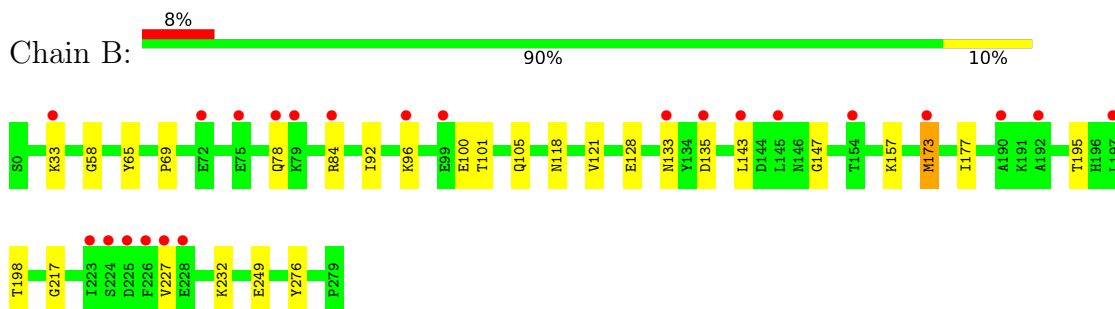
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	69.59Å 114.68Å 127.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.19 – 1.74 34.19 – 1.74	Depositor EDS
% Data completeness (in resolution range)	98.9 (34.19-1.74) 96.4 (34.19-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 1.74Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.166 , 0.207 0.179 , 0.214	Depositor DCC
R_{free} test set	2001 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.899	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.9	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.018 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.027 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4581	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.42	0/2177	1.29	8/2963 (0.3%)
2	B	0.42	0/2164	1.04	4/2947 (0.1%)
All	All	0.42	0/4341	1.17	12/5910 (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	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	GLU	OE1-CD-OE2	-35.26	80.99	123.30
2	B	128	GLU	OE1-CD-OE2	-35.19	81.07	123.30
1	A	52	GLU	OE1-CD-OE2	-29.93	87.39	123.30
2	B	128	GLU	CG-CD-OE1	22.34	162.97	118.30
1	A	128	GLU	CG-CD-OE1	21.87	162.03	118.30
1	A	52	GLU	CG-CD-OE1	21.32	160.94	118.30
2	B	128	GLU	CG-CD-OE2	-17.76	82.77	118.30
1	A	128	GLU	CG-CD-OE2	-17.53	83.23	118.30
1	A	52	GLU	CG-CD-OE2	-16.43	85.43	118.30
1	A	135	ASP	CB-CG-OD2	-8.38	110.76	118.30
2	B	173	MET	CB-CG-SD	-5.80	95.00	112.40
1	A	135	ASP	CB-CG-OD1	5.32	123.09	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	GLU	Sidechain

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	2127	0	2085	18	1
2	B	2115	0	2068	23	1
3	A	48	0	26	2	0
3	B	48	0	26	2	0
4	A	124	0	0	0	0
4	B	119	0	0	0	0
All	All	4581	0	4205	40	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (40) 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)
2:B:173:MET:HE1	2:B:276:TYR:CD1	1.97	0.99
1:A:75:GLU:HG2	1:A:79:LYS:HE2	1.71	0.72
1:A:123:TRP:CE3	1:A:186:PRO:HG2	2.26	0.71
1:A:217:GLY:O	3:A:301:NDP:H42N	1.93	0.68
2:B:96:LYS:O	2:B:100:GLU:HG3	1.96	0.64
2:B:101:THR:O	2:B:105:GLN:HG3	1.97	0.64
2:B:217:GLY:O	3:B:301:NDP:H42N	1.96	0.64
2:B:33:LYS:HG2	2:B:58:GLY:HA3	1.81	0.62
2:B:78:GLN:OE1	2:B:84:ARG:HA	2.02	0.58
1:A:172:SER:HB2	3:A:301:NDP:H6N	1.89	0.55
2:B:173:MET:CE	2:B:276:TYR:CD1	2.80	0.55
1:A:153:HIS:CD2	1:A:157:LYS:HZ1	2.30	0.50
1:A:169:ILE:HB	1:A:213:THR:HG22	1.92	0.49
1:A:133:ASN:OD1	1:A:135:ASP:OD2	2.30	0.49
2:B:121:VAL:HG13	2:B:143:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:VAL:HG23	2:B:232:LYS:HG3	1.95	0.49
1:A:263:THR:OG1	2:B:249:GLU:HG2	2.13	0.48
1:A:18:LYS:HA	1:A:18:LYS:HD2	1.53	0.48
1:A:78:GLN:HG2	1:A:83:VAL:O	2.15	0.47
2:B:173:MET:HE3	2:B:276:TYR:HB3	1.97	0.47
1:A:133:ASN:CG	1:A:135:ASP:OD2	2.53	0.47
2:B:173:MET:HB2	2:B:173:MET:HE2	1.63	0.47
2:B:173:MET:SD	2:B:217:GLY:HA2	2.54	0.47
2:B:33:LYS:HG2	2:B:58:GLY:CA	2.45	0.46
1:A:101:THR:O	1:A:105:GLN:HG3	2.15	0.45
1:A:123:TRP:CZ3	1:A:186:PRO:HG2	2.51	0.45
2:B:118:ASN:O	3:B:301:NDP:H4D	2.17	0.45
2:B:65:TYR:CD1	2:B:69:PRO:HA	2.53	0.44
1:A:232:LYS:HD3	1:A:244:GLU:OE1	2.17	0.44
1:A:182:GLN:O	1:A:182:GLN:HG2	2.17	0.44
1:A:198:ALA:CB	1:A:213:THR:HG23	2.49	0.43
2:B:173:MET:HE2	2:B:177:ILE:CD1	2.48	0.43
2:B:173:MET:CE	2:B:177:ILE:HD11	2.50	0.42
2:B:92:ILE:HG22	2:B:147:GLY:HA3	2.01	0.42
1:A:133:ASN:ND2	1:A:135:ASP:OD2	2.53	0.41
2:B:173:MET:HE2	2:B:177:ILE:HD11	2.02	0.41
1:A:173:ILE:O	1:A:177:ILE:HG12	2.20	0.41
2:B:195:THR:O	2:B:198:THR:HB	2.20	0.41
2:B:133:ASN:ND2	2:B:135:ASP:HB2	2.37	0.40
2:B:33:LYS:CG	2:B:58:GLY:HA3	2.50	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASP:OD2	2:B:157:LYS:NZ[4_555]	2.06	0.14

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/280 (99%)	269 (97%)	9 (3%)	0	100	100
2	B	278/280 (99%)	265 (95%)	13 (5%)	0	100	100
All	All	556/560 (99%)	534 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/229 (100%)	229 (100%)	0	100	100
2	B	223/224 (100%)	223 (100%)	0	100	100
All	All	452/453 (100%)	452 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
2	B	142	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	#$|Z| > 2$
3	NDP	B	301	-	45,52,52	4.01	24 (53%)	53,80,80	3.05	6 (11%)
3	NDP	A	301	-	45,52,52	3.98	23 (51%)	53,80,80	3.00	10 (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
3	NDP	B	301	-	-	11/30/77/77	0/5/5/5
3	NDP	A	301	-	-	12/30/77/77	0/5/5/5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	NDP	C6N-C5N	12.20	1.55	1.33
3	A	301	NDP	C6N-C5N	11.97	1.54	1.33
3	B	301	NDP	C3D-C4D	-9.83	1.27	1.53
3	A	301	NDP	C3D-C4D	-9.82	1.27	1.53
3	B	301	NDP	C3B-C4B	-8.31	1.31	1.53
3	B	301	NDP	C2D-C1D	-8.31	1.26	1.53
3	A	301	NDP	C2D-C1D	-8.25	1.27	1.53
3	A	301	NDP	C3B-C4B	-8.13	1.32	1.53
3	A	301	NDP	O4B-C4B	7.34	1.61	1.45
3	B	301	NDP	O4B-C4B	6.86	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	NDP	C2N-C3N	6.10	1.52	1.34
3	B	301	NDP	O4B-C1B	-6.04	1.32	1.41
3	A	301	NDP	O4B-C1B	-5.88	1.32	1.41
3	A	301	NDP	C2N-C3N	5.80	1.51	1.34
3	B	301	NDP	O4D-C1D	5.39	1.54	1.42
3	A	301	NDP	O4D-C1D	5.12	1.54	1.42
3	A	301	NDP	P2B-O2B	4.74	1.68	1.59
3	B	301	NDP	C7N-N7N	4.64	1.45	1.33
3	B	301	NDP	P2B-O2B	4.57	1.67	1.59
3	A	301	NDP	O4D-C4D	4.52	1.55	1.45
3	A	301	NDP	C7N-N7N	4.46	1.45	1.33
3	A	301	NDP	C2D-C3D	4.44	1.65	1.53
3	B	301	NDP	O4D-C4D	4.42	1.54	1.45
3	B	301	NDP	C2D-C3D	4.30	1.65	1.53
3	A	301	NDP	C6A-N6A	4.20	1.49	1.34
3	B	301	NDP	C6A-N6A	4.12	1.49	1.34
3	B	301	NDP	C5D-C4D	3.10	1.61	1.51
3	B	301	NDP	C5A-C4A	-3.06	1.32	1.40
3	A	301	NDP	C5D-C4D	2.94	1.60	1.51
3	A	301	NDP	C5A-C4A	-2.91	1.33	1.40
3	A	301	NDP	O7N-C7N	-2.71	1.18	1.24
3	B	301	NDP	C4N-C5N	2.69	1.55	1.48
3	B	301	NDP	C6N-N1N	2.63	1.43	1.37
3	B	301	NDP	O3B-C3B	2.62	1.49	1.43
3	A	301	NDP	C4N-C5N	2.60	1.55	1.48
3	A	301	NDP	O3B-C3B	2.59	1.49	1.43
3	A	301	NDP	C6N-N1N	2.52	1.43	1.37
3	B	301	NDP	C4N-C3N	2.48	1.54	1.49
3	B	301	NDP	O7N-C7N	-2.41	1.18	1.24
3	A	301	NDP	PA-O5B	2.33	1.68	1.59
3	A	301	NDP	C4N-C3N	2.33	1.54	1.49
3	B	301	NDP	O2D-C2D	2.19	1.48	1.43
3	A	301	NDP	O2D-C2D	2.18	1.48	1.43
3	B	301	NDP	O3D-C3D	2.16	1.48	1.43
3	B	301	NDP	O2B-C2B	-2.15	1.36	1.44
3	A	301	NDP	O3D-C3D	2.07	1.47	1.43
3	B	301	NDP	PN-O5D	2.05	1.67	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	NDP	C5A-C6A-N6A	15.88	144.49	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	NDP	C5A-C6A-N6A	15.69	144.20	120.35
3	B	301	NDP	N6A-C6A-N1A	-10.98	95.78	118.57
3	A	301	NDP	N6A-C6A-N1A	-10.67	96.43	118.57
3	B	301	NDP	N3A-C2A-N1A	-5.64	119.87	128.68
3	A	301	NDP	N3A-C2A-N1A	-5.57	119.97	128.68
3	B	301	NDP	C1B-N9A-C4A	4.72	134.93	126.64
3	A	301	NDP	C1B-N9A-C4A	4.08	133.81	126.64
3	A	301	NDP	C4D-O4D-C1D	-3.18	102.45	109.47
3	B	301	NDP	C4D-O4D-C1D	-2.93	103.00	109.47
3	A	301	NDP	O4D-C1D-N1N	-2.46	103.25	108.06
3	A	301	NDP	C3N-C2N-N1N	-2.38	119.70	123.10
3	A	301	NDP	PN-O3-PA	-2.12	125.54	132.83
3	A	301	NDP	O7N-C7N-C3N	-2.10	116.94	120.90
3	B	301	NDP	C3B-C2B-C1B	-2.09	98.95	102.89
3	A	301	NDP	O4D-C1D-C2D	-2.07	102.12	106.64

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	NDP	PN-O3-PA-O5B
3	A	301	NDP	C5D-O5D-PN-O1N
3	B	301	NDP	C5B-O5B-PA-O2A
3	B	301	NDP	C2B-O2B-P2B-O1X
3	B	301	NDP	C2B-O2B-P2B-O3X
3	B	301	NDP	O4B-C4B-C5B-O5B
3	B	301	NDP	C3B-C4B-C5B-O5B
3	A	301	NDP	O4D-C1D-N1N-C6N
3	A	301	NDP	O4B-C4B-C5B-O5B
3	B	301	NDP	O4D-C1D-N1N-C6N
3	A	301	NDP	C5B-O5B-PA-O3
3	B	301	NDP	C5B-O5B-PA-O3
3	B	301	NDP	C5D-O5D-PN-O3
3	B	301	NDP	PA-O3-PN-O1N
3	A	301	NDP	C5B-O5B-PA-O1A
3	A	301	NDP	C5B-O5B-PA-O2A
3	A	301	NDP	C5D-O5D-PN-O2N
3	B	301	NDP	C5B-O5B-PA-O1A
3	B	301	NDP	C5D-O5D-PN-O2N
3	A	301	NDP	C3B-C4B-C5B-O5B
3	A	301	NDP	C2B-O2B-P2B-O2X
3	A	301	NDP	C5D-O5D-PN-O3

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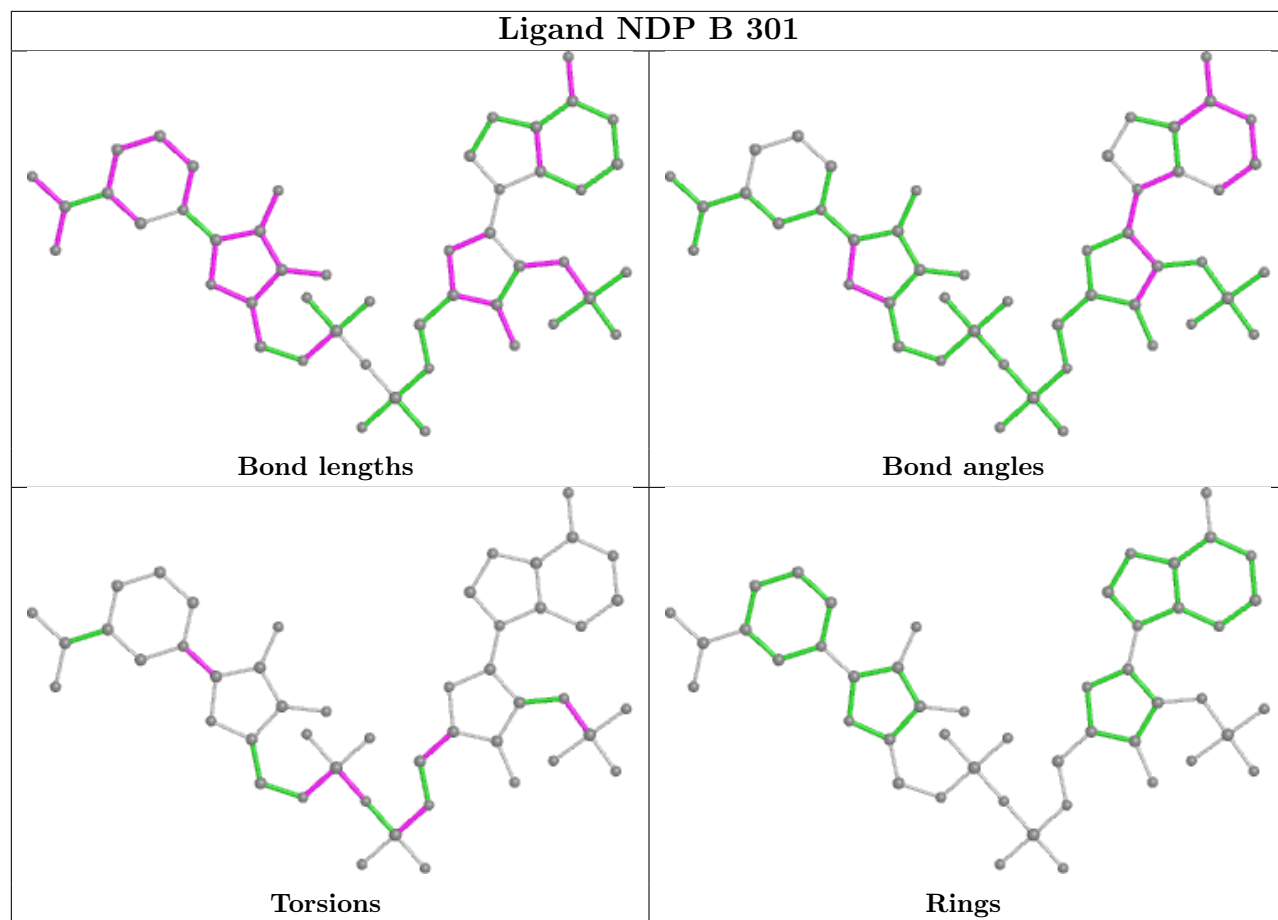| Mol	Chain	Res	Type	Atoms
3	A	301	NDP	PA-O3-PN-O2N

There are no ring outliers.

2 monomers are involved in 4 short contacts:

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

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP A 301

Bond lengths

Bond angles

Torsions

Rings
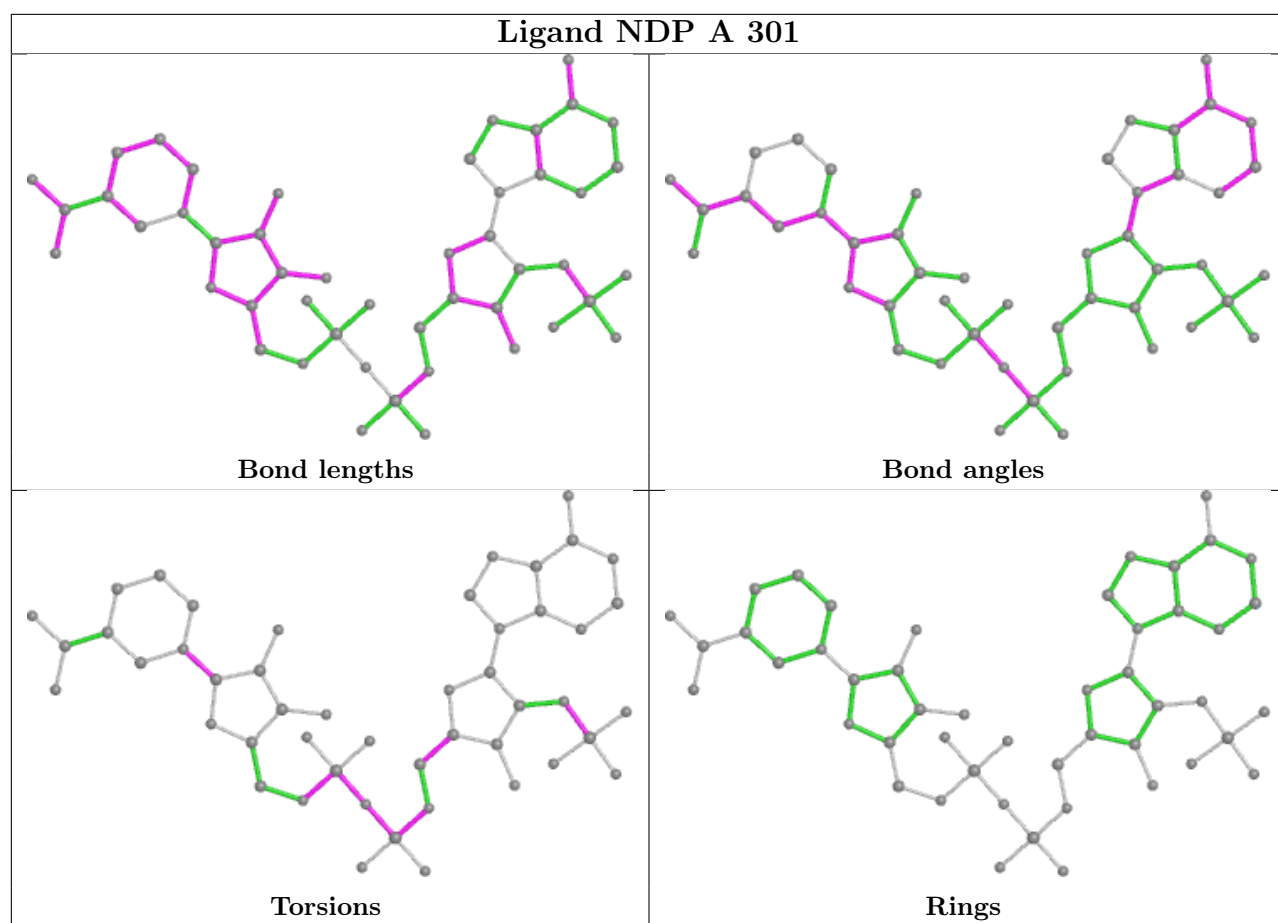
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	280/280 (100%)	0.63	21 (7%)	14	18	20, 36, 57, 79	0
2	B	280/280 (100%)	0.53	23 (8%)	11	15	19, 36, 57, 83	1 (0%)
All	All	560/560 (100%)	0.58	44 (7%)	12	16	19, 36, 57, 83	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	226	PHE	9.7
1	A	226	PHE	9.2
2	B	223	ILE	7.4
1	A	224	THR	6.8
1	A	82	GLY	4.8
1	A	223	ILE	4.5
2	B	133	ASN	4.2
1	A	84	HIS	3.9
2	B	96	LYS	3.5
2	B	227	VAL	3.3
1	A	72	GLU	3.3
2	B	75	GLU	3.2
1	A	225	ASP	3.2
2	B	72	GLU	3.1
2	B	143	LEU	3.1
1	A	79	LYS	3.0
2	B	135	ASP	3.0
2	B	154	THR	2.9
2	B	79	LYS	2.9
2	B	84	ARG	2.9
2	B	225	ASP	2.8
1	A	170	THR	2.7
2	B	145	LEU	2.7
1	A	132	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	81	TYR	2.7
1	A	135	ASP	2.6
1	A	194	CYS	2.6
2	B	192	ALA	2.5
2	B	228	GLU	2.4
1	A	192	ALA	2.4
2	B	197	LEU	2.4
1	A	141	ILE	2.3
1	A	190	ALA	2.3
2	B	173	MET	2.2
1	A	220	ASP	2.2
2	B	33	LYS	2.2
1	A	78	GLN	2.1
1	A	173	ILE	2.1
2	B	78	GLN	2.1
1	A	75	GLU	2.1
1	A	0	SER	2.1
2	B	224	SER	2.0
2	B	190	ALA	2.0
2	B	99	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

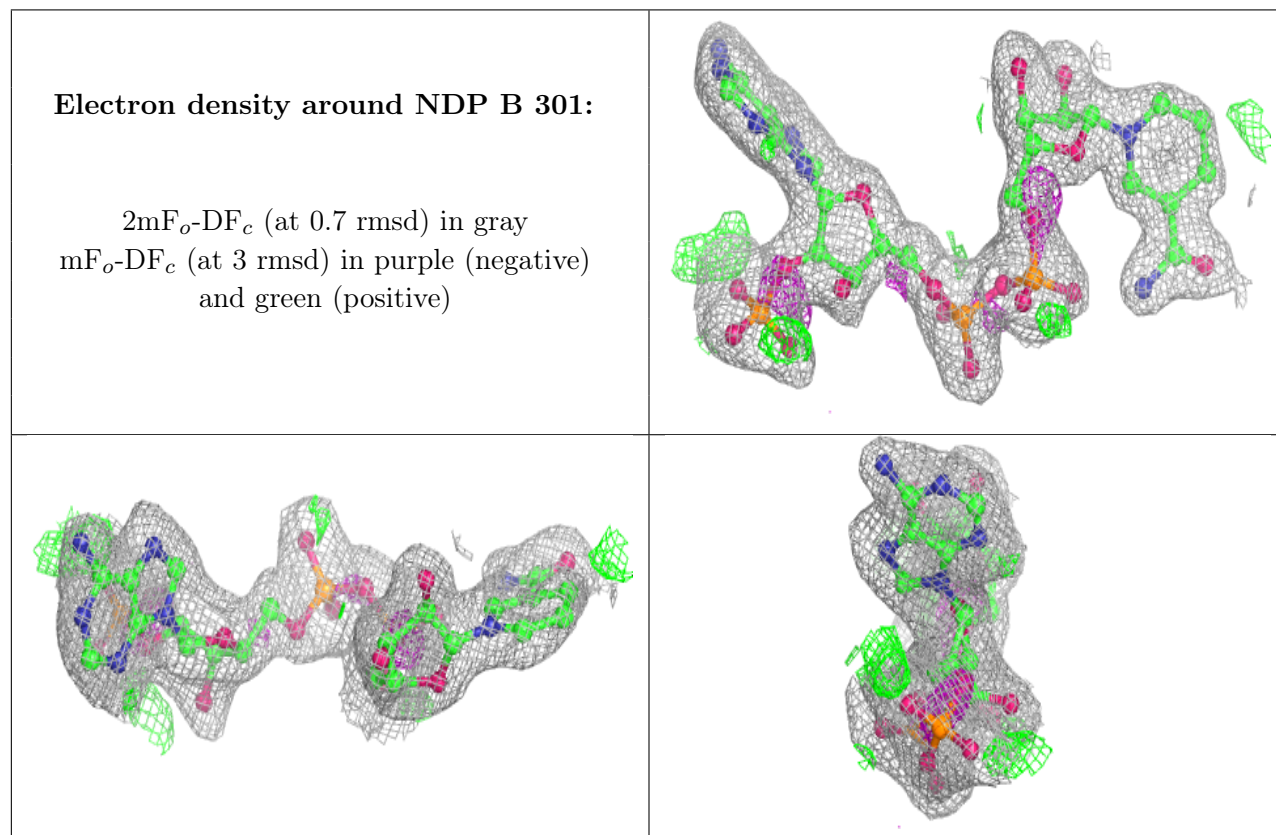There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

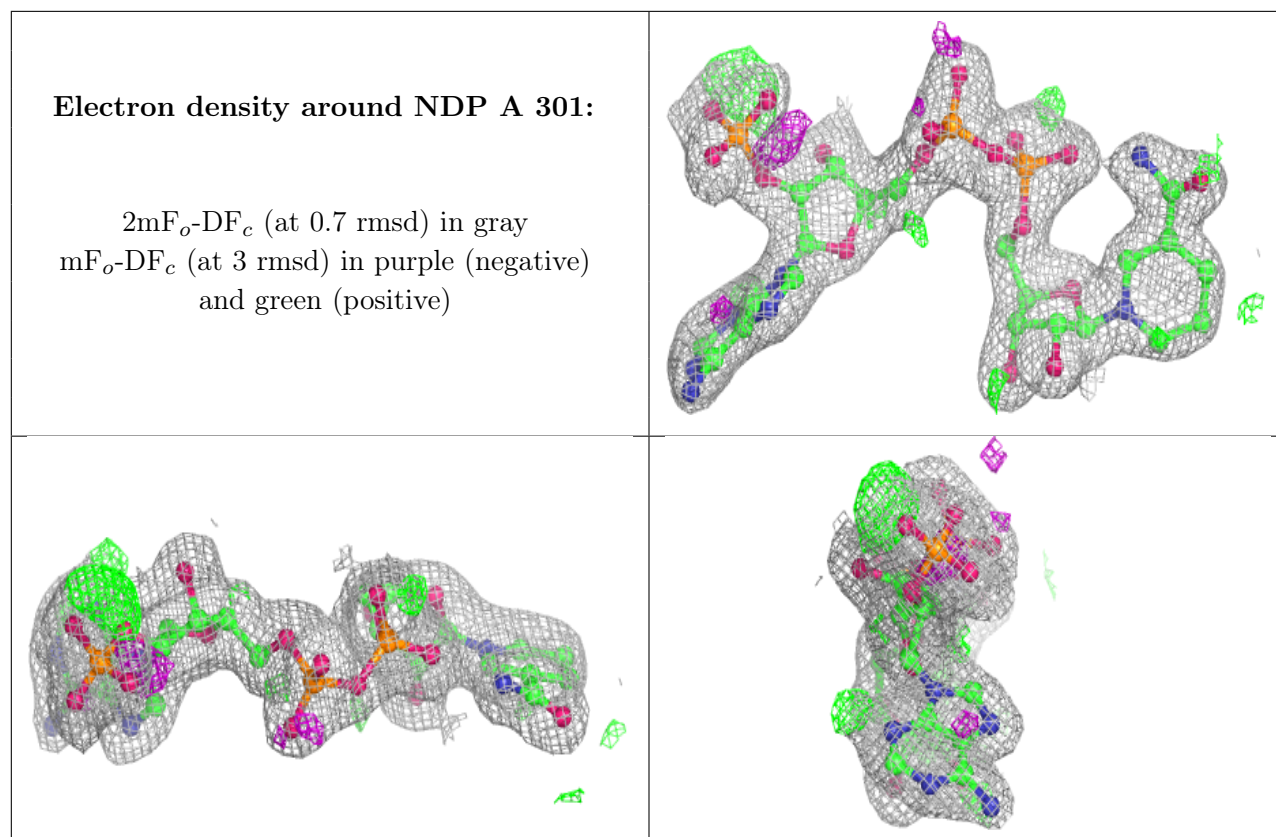## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NDP	B	301	48/48	0.93	0.10	28,33,39,41	0
3	NDP	A	301	48/48	0.94	0.10	27,35,40,42	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 B 301:

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

Electron density around NDP A 301:

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

6.5 Other polymers (i)

There are no such residues in this entry.