



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 01:26 AM EDT

PDB ID : 1PNN  
Title : PEPTIDE NUCLEIC ACID (PNA) COMPLEXED WITH DNA  
Authors : Betts, L.; Veal, J.M.  
Deposited on : 1995-10-13  
Resolution : 2.50 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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

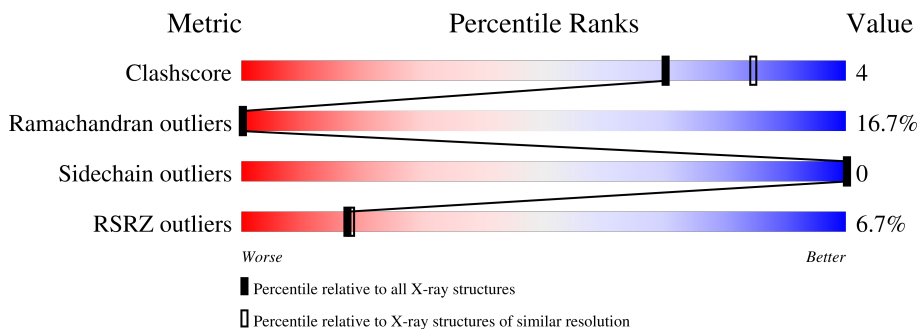
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	24	
1	C	24	
2	B	9	
2	D	9	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1983 atoms, of which 818 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 DNA chain called PNA (NH<sub>2</sub>-P(\*C\*T\*C\*T\*T\*C\*T\*T\*C-HIS-GLY-SER-SER-GLY-HIS-C\*T\*T\*C\*T\*T\*C\*T\*T\*C)-COOH).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	A	24	Total	C	H	I	N	O	0	0	0
			648	211	273	1	90	73			
1	C	24	Total	C	H	I	N	O	0	0	0
			648	211	273	1	90	73			

- Molecule 2 is a DNA chain called DNA (5'-D(GP\*AP\*AP\*GP\*AP\*AP\*GP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	B	9	Total	C	H	N	O	P	0	0	0
			291	90	101	45	47	8			
2	D	9	Total	C	H	N	O	P	0	0	0
			291	90	101	45	47	8			

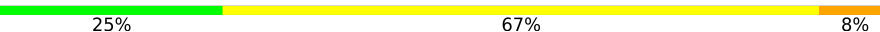
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	A	10	Total	H	O	0	0
			30	20	10		
3	B	4	Total	H	O	0	0
			12	8	4		
3	C	12	Total	H	O	0	0
			36	24	12		
3	D	9	Total	H	O	0	0
			27	18	9		

### 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.

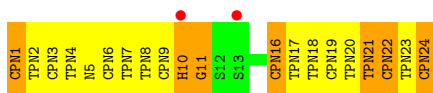
- Molecule 1: PNA (NH<sub>2</sub>-P(\*C\*T\*C\*T\*T\*C\*T\*T\*C-HIS-GLY-SER-SER-GLY-HIS-C\*T\*T\*C\*T\*T\*C\*T\*C)-COOH)

Chain A: 




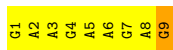
- Molecule 1: PNA (NH<sub>2</sub>-P(\*C\*T\*C\*T\*T\*C\*T\*T\*C-HIS-GLY-SER-SER-GLY-HIS-C\*T\*T\*C\*T\*T\*C\*T\*C)-COOH)

Chain C: 

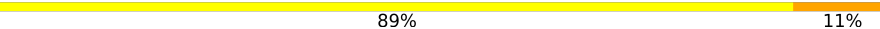


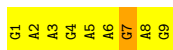
- Molecule 2: DNA (5'-D(GP\*AP\*AP\*GP\*AP\*AP\*GP\*AP\*G)-3')

Chain B: 



- Molecule 2: DNA (5'-D(GP\*AP\*AP\*GP\*AP\*AP\*GP\*AP\*G)-3')

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.38Å 73.38Å 141.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.50 32.56 – 2.17	Depositor EDS
% Data completeness (in resolution range)	95.0 (6.00-2.50) 84.7 (32.56-2.17)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.46 (at 2.18Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.187 , 0.235 0.187 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	1983	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CPN, TPN, IPN

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	0.79	0/41	1.11	0/53
1	C	1.15	0/41	1.94	2/53 (3.8%)
2	B	2.47	12/216 (5.6%)	3.11	39/333 (11.7%)
2	D	2.44	15/216 (6.9%)	3.10	43/333 (12.9%)
All	All	2.28	27/514 (5.3%)	2.94	84/772 (10.9%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	9	DG	N1-C2	-8.86	1.30	1.37
2	D	4	DG	N1-C2	-7.51	1.31	1.37
2	D	6	DA	N3-C4	7.02	1.39	1.34
2	D	7	DG	N1-C2	-6.85	1.32	1.37
2	B	7	DG	N1-C2	-6.65	1.32	1.37
2	B	7	DG	C2-N2	-6.23	1.28	1.34
2	D	5	DA	C6-N1	-6.11	1.31	1.35
2	D	4	DG	C2-N2	-6.08	1.28	1.34
2	B	9	DG	C2-N2	-6.06	1.28	1.34
2	D	8	DA	N3-C4	5.65	1.38	1.34
2	D	9	DG	N1-C2	-5.64	1.33	1.37
2	B	1	DG	N1-C2	-5.61	1.33	1.37
2	D	1	DG	C2-N2	-5.57	1.28	1.34
2	B	2	DA	C6-N6	-5.57	1.29	1.33
2	D	3	DA	N3-C4	5.50	1.38	1.34
2	D	9	DG	C2-N2	-5.46	1.29	1.34
2	D	7	DG	C2-N2	-5.46	1.29	1.34
2	D	2	DA	N3-C4	5.42	1.38	1.34
2	D	5	DA	N3-C4	5.40	1.38	1.34
2	B	1	DG	C2-N2	-5.35	1.29	1.34
2	B	2	DA	C6-N1	-5.33	1.31	1.35
2	B	4	DG	N1-C2	-5.31	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	DG	C6-N1	-5.25	1.35	1.39
2	B	8	DA	C4'-O4'	-5.12	1.40	1.45
2	B	5	DA	C6-N6	-5.12	1.29	1.33
2	B	4	DG	C2-N2	-5.07	1.29	1.34
2	D	2	DA	C6-N6	-5.06	1.29	1.33

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	DA	N1-C6-N6	-13.18	110.69	118.60
2	B	2	DA	N1-C6-N6	-12.07	111.36	118.60
2	B	5	DA	N1-C6-N6	-10.65	112.21	118.60
2	D	5	DA	N1-C6-N6	-10.51	112.29	118.60
2	D	2	DA	C5-C6-N1	10.48	122.94	117.70
2	B	5	DA	C5-C6-N1	10.24	122.82	117.70
2	D	2	DA	C4-C5-C6	-9.95	112.02	117.00
2	D	5	DA	C5-C6-N1	9.85	122.63	117.70
2	D	6	DA	N1-C6-N6	-9.55	112.87	118.60
2	B	5	DA	C4-C5-C6	-9.40	112.30	117.00
2	D	8	DA	C5-C6-N1	9.26	122.33	117.70
2	D	5	DA	C4-C5-C6	-9.22	112.39	117.00
2	B	9	DG	O4'-C4'-C3'	-9.04	100.58	106.00
2	B	6	DA	N1-C6-N6	-8.98	113.21	118.60
2	B	2	DA	C5-C6-N1	8.97	122.18	117.70
2	B	2	DA	C4-C5-C6	-8.93	112.53	117.00
2	B	9	DG	N1-C6-O6	-8.66	114.70	119.90
2	D	6	DA	C4-C5-C6	-8.64	112.68	117.00
2	B	3	DA	N1-C6-N6	-8.60	113.44	118.60
2	B	7	DG	C4'-C3'-C2'	-8.32	95.61	103.10
2	B	6	DA	C4-C5-C6	-8.21	112.89	117.00
2	D	7	DG	C4'-C3'-C2'	-8.20	95.72	103.10
2	D	3	DA	N1-C6-N6	-8.17	113.69	118.60
2	D	8	DA	C4-C5-C6	-8.01	113.00	117.00
2	D	7	DG	N1-C6-O6	-7.91	115.15	119.90
2	B	3	DA	C4-C5-C6	-7.75	113.12	117.00
2	D	2	DA	N1-C2-N3	-7.73	125.44	129.30
2	B	8	DA	P-O3'-C3'	7.51	128.71	119.70
2	B	1	DG	C5-C6-N1	7.37	115.18	111.50
2	B	2	DA	N1-C2-N3	-7.28	125.66	129.30
2	B	6	DA	N1-C2-N3	-7.19	125.70	129.30
2	D	3	DA	C4-C5-C6	-7.19	113.41	117.00
1	C	11	GLY	N-CA-C	7.13	130.94	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	DG	C5-C6-N1	7.13	115.06	111.50
2	B	4	DG	N1-C6-O6	-7.04	115.68	119.90
1	C	10	HIS	C-N-CA	6.96	136.91	122.30
2	D	1	DG	O4'-C1'-N9	6.54	112.58	108.00
2	B	2	DA	C6-C5-N7	6.52	136.87	132.30
2	B	8	DA	C4-C5-C6	-6.52	113.74	117.00
2	B	3	DA	C5-C6-N1	6.52	120.96	117.70
2	D	6	DA	C6-C5-N7	6.51	136.86	132.30
2	B	8	DA	N1-C2-N3	-6.49	126.06	129.30
2	B	5	DA	C4'-C3'-C2'	-6.43	97.31	103.10
2	B	7	DG	C5-C6-N1	6.43	114.71	111.50
2	B	9	DG	N1-C2-N3	6.42	127.75	123.90
2	B	9	DG	C5-C6-N1	6.39	114.69	111.50
2	D	6	DA	C4'-C3'-C2'	-6.38	97.36	103.10
2	D	9	DG	N1-C6-O6	-6.34	116.09	119.90
2	B	8	DA	C5-C6-N1	6.29	120.84	117.70
2	B	7	DG	N1-C6-O6	-6.28	116.13	119.90
2	D	5	DA	C4'-C3'-C2'	-6.27	97.46	103.10
2	D	2	DA	C6-C5-N7	6.20	136.64	132.30
2	D	3	DA	C5-C6-N1	6.14	120.77	117.70
2	D	6	DA	C5-C6-N1	6.11	120.75	117.70
2	D	8	DA	O4'-C1'-N9	-6.10	103.73	108.00
2	D	7	DG	C5-C6-N1	6.09	114.54	111.50
2	B	1	DG	O4'-C1'-C2'	6.07	110.76	105.90
2	B	6	DA	C4'-C3'-C2'	-6.01	97.69	103.10
2	D	1	DG	C5-C6-N1	5.99	114.50	111.50
2	D	1	DG	N3-C2-N2	-5.99	115.71	119.90
2	B	6	DA	C5-C6-N1	5.97	120.68	117.70
2	B	6	DA	C6-C5-N7	5.93	136.45	132.30
2	B	5	DA	C6-C5-N7	5.91	136.44	132.30
2	D	9	DG	C4-C5-N7	-5.89	108.44	110.80
2	D	9	DG	C6-C5-N7	5.67	133.80	130.40
2	D	4	DG	N1-C6-O6	-5.65	116.51	119.90
2	D	9	DG	N3-C2-N2	-5.64	115.95	119.90
2	D	4	DG	C4'-C3'-C2'	-5.62	98.04	103.10
2	D	8	DA	N1-C6-N6	-5.59	115.25	118.60
2	B	5	DA	N1-C2-N3	-5.55	126.53	129.30
2	D	5	DA	C6-C5-N7	5.53	136.17	132.30
2	D	9	DG	C5-C6-N1	5.51	114.26	111.50
2	B	4	DG	C4'-C3'-C2'	-5.35	98.28	103.10
2	B	8	DA	C4'-C3'-C2'	-5.35	98.29	103.10
2	D	4	DG	C5-C6-N1	5.32	114.16	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	DA	C2-N3-C4	5.30	113.25	110.60
2	B	4	DG	C6-N1-C2	-5.20	121.98	125.10
2	D	5	DA	N1-C2-N3	-5.18	126.71	129.30
2	D	1	DG	C8-N9-C4	-5.17	104.33	106.40
2	D	1	DG	N3-C4-C5	-5.12	126.04	128.60
2	D	6	DA	N1-C2-N3	-5.11	126.74	129.30
2	D	1	DG	C6-N1-C2	-5.10	122.04	125.10
2	D	9	DG	N1-C2-N3	5.05	126.93	123.90
2	B	9	DG	C6-C5-N7	5.01	133.41	130.40

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	375	273	186	3	0
1	C	375	273	186	5	0
2	B	190	101	90	1	0
2	D	190	101	93	1	0
3	A	10	20	0	0	0
3	B	4	8	0	0	0
3	C	12	24	0	1	0
3	D	9	18	0	0	0
All	All	1165	818	555	6	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 4.

All (6) 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:24:CPN:OXT	1:C:1:CPN:N	2.47	0.48
1:C:21:TPN:HM51	3:C:152:HOH:O	2.13	0.47
1:A:24:CPN:N3	2:B:9:DG:N7	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:CPN:O	1:C:16:CPN:C2'	2.66	0.43
1:A:1:CPN:N	1:C:24:CPN:OXT	2.51	0.43
1:C:22:CPN:N3	2:D:7:DG:N7	2.68	0.42

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

36 non-standard protein/DNA/RNA residues 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
1	TPN	C	18	1,2	19,19,20	1.37	3 (15%)	23,25,27	1.74	7 (30%)
1	TPN	C	7	1,2	19,19,20	1.22	4 (21%)	23,25,27	1.82	6 (26%)
1	TPN	A	8	1,2	19,19,20	0.91	1 (5%)	23,25,27	1.74	4 (17%)
1	CPN	A	19	1,2	18,18,19	1.20	3 (16%)	20,23,25	1.62	5 (25%)
1	TPN	A	17	1,2	19,19,20	1.26	3 (15%)	23,25,27	2.12	7 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CPN	C	1	1,2	18,18,19	1.61	5 (27%)	20,23,25	2.16	11 (55%)
1	TPN	C	4	1,2	19,19,20	1.08	1 (5%)	23,25,27	1.95	9 (39%)
1	CPN	C	16	1,2	18,18,19	1.32	3 (16%)	20,23,25	1.54	4 (20%)
1	CPN	C	9	1,2	18,18,19	1.10	1 (5%)	20,23,25	2.48	10 (50%)
1	CPN	C	6	1,2	18,18,19	1.26	4 (22%)	20,23,25	1.94	6 (30%)
1	CPN	C	22	1,2	18,18,19	1.43	3 (16%)	20,23,25	1.91	7 (35%)
1	TPN	C	8	1,2	19,19,20	0.89	0	23,25,27	1.79	4 (17%)
1	TPN	A	2	1,2	19,19,20	1.03	2 (10%)	23,25,27	1.69	6 (26%)
1	IPN	A	5	1,2	19,19,20	3.27	3 (15%)	23,25,27	2.30	10 (43%)
1	TPN	A	7	1,2	19,19,20	1.04	1 (5%)	23,25,27	1.77	4 (17%)
1	TPN	A	21	1,2	19,19,20	1.45	3 (15%)	23,25,27	1.78	7 (30%)
1	TPN	C	23	1,2	19,19,20	1.25	3 (15%)	23,25,27	1.93	7 (30%)
1	TPN	C	17	1,2	19,19,20	1.16	2 (10%)	23,25,27	2.10	10 (43%)
1	CPN	A	22	1,2	18,18,19	1.58	3 (16%)	20,23,25	2.02	7 (35%)
1	CPN	A	6	1,2	18,18,19	1.14	3 (16%)	20,23,25	2.10	8 (40%)
1	CPN	A	24	1,2	19,19,19	1.28	3 (15%)	24,25,25	2.07	5 (20%)
1	IPN	C	5	1,2	19,19,20	3.23	3 (15%)	23,25,27	2.19	10 (43%)
1	TPN	C	21	1,2	19,19,20	1.52	3 (15%)	23,25,27	1.95	10 (43%)
1	CPN	A	3	1,2	18,18,19	1.11	1 (5%)	20,23,25	1.98	10 (50%)
1	CPN	A	9	1,2	18,18,19	1.18	2 (11%)	20,23,25	1.82	7 (35%)
1	TPN	C	2	1,2	19,19,20	0.97	1 (5%)	23,25,27	1.69	7 (30%)
1	CPN	C	24	1,2	19,19,19	1.57	3 (15%)	24,25,25	1.94	9 (37%)
1	CPN	C	19	1,2	18,18,19	1.38	3 (16%)	20,23,25	1.43	5 (25%)
1	TPN	A	20	1,2	19,19,20	1.04	2 (10%)	23,25,27	1.98	7 (30%)
1	TPN	A	18	1,2	19,19,20	1.35	3 (15%)	23,25,27	1.91	9 (39%)
1	CPN	C	3	1,2	18,18,19	1.15	2 (11%)	20,23,25	2.17	10 (50%)
1	TPN	A	4	1,2	19,19,20	1.03	2 (10%)	23,25,27	1.88	9 (39%)
1	CPN	A	1	1,2	18,18,19	1.37	3 (16%)	20,23,25	2.30	7 (35%)
1	CPN	A	16	1	18,18,19	1.21	2 (11%)	20,23,25	2.31	8 (40%)
1	TPN	C	20	1,2	19,19,20	1.17	2 (10%)	23,25,27	1.85	6 (26%)
1	TPN	A	23	1,2	19,19,20	1.19	2 (10%)	23,25,27	2.00	7 (30%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPN	C	18	1,2	-	0/13/14/15	0/1/1/1
1	TPN	C	7	1,2	-	0/13/14/15	0/1/1/1
1	TPN	A	8	1,2	-	0/13/14/15	0/1/1/1
1	CPN	A	19	1,2	-	0/13/14/15	0/1/1/1
1	TPN	A	17	1,2	-	1/13/14/15	0/1/1/1
1	CPN	C	1	1,2	-	0/13/14/15	0/1/1/1
1	TPN	C	4	1,2	-	0/13/14/15	0/1/1/1
1	CPN	C	16	1,2	-	0/13/14/15	0/1/1/1
1	CPN	C	9	1,2	-	2/13/14/15	0/1/1/1
1	CPN	C	6	1,2	-	0/13/14/15	0/1/1/1
1	CPN	C	22	1,2	-	0/13/14/15	0/1/1/1
1	TPN	C	8	1,2	-	0/13/14/15	0/1/1/1
1	TPN	A	2	1,2	-	0/13/14/15	0/1/1/1
1	IPN	A	5	1,2	-	0/13/14/15	0/1/1/1
1	TPN	A	7	1,2	-	0/13/14/15	0/1/1/1
1	TPN	A	21	1,2	-	0/13/14/15	0/1/1/1
1	TPN	C	23	1,2	-	0/13/14/15	0/1/1/1
1	TPN	C	17	1,2	-	1/13/14/15	0/1/1/1
1	CPN	A	22	1,2	-	0/13/14/15	0/1/1/1
1	CPN	A	6	1,2	-	0/13/14/15	0/1/1/1
1	CPN	A	24	1,2	-	0/15/15/15	0/1/1/1
1	IPN	C	5	1,2	-	0/13/14/15	0/1/1/1
1	TPN	C	21	1,2	-	0/13/14/15	0/1/1/1
1	CPN	A	3	1,2	-	0/13/14/15	0/1/1/1
1	CPN	A	9	1,2	-	2/13/14/15	0/1/1/1
1	TPN	C	2	1,2	-	0/13/14/15	0/1/1/1
1	CPN	C	24	1,2	-	0/15/15/15	0/1/1/1
1	CPN	C	19	1,2	-	0/13/14/15	0/1/1/1
1	TPN	A	20	1,2	-	0/13/14/15	0/1/1/1
1	TPN	A	18	1,2	-	0/13/14/15	0/1/1/1
1	CPN	C	3	1,2	-	0/13/14/15	0/1/1/1
1	TPN	A	4	1,2	-	0/13/14/15	0/1/1/1
1	CPN	A	1	1,2	-	0/13/14/15	0/1/1/1
1	CPN	A	16	1	-	4/13/14/15	0/1/1/1
1	TPN	C	20	1,2	-	0/13/14/15	0/1/1/1
1	TPN	A	23	1,2	-	0/13/14/15	0/1/1/1

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	IPN	C5-I5	-13.05	1.69	2.08
1	C	5	IPN	C5-I5	-12.67	1.70	2.08
1	A	22	CPN	C8 <sup>2</sup> -N1	4.50	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	5	IPN	C8'-N1	4.36	1.51	1.46
1	C	1	CPN	C8'-C7'	3.79	1.58	1.53
1	C	21	TPN	C4-N3	-3.64	1.32	1.38
1	C	24	CPN	C4-N3	-3.56	1.27	1.34
1	A	21	TPN	C8'-N1	3.42	1.50	1.46
1	A	18	TPN	C4-N3	-3.31	1.32	1.38
1	C	24	CPN	C8'-N1	3.22	1.50	1.46
1	C	18	TPN	C4-N3	-3.19	1.32	1.38
1	C	22	CPN	C8'-N1	3.19	1.50	1.46
1	A	18	TPN	C8'-N1	3.06	1.50	1.46
1	C	19	CPN	C4-N3	-2.98	1.28	1.34
1	C	5	IPN	C2-N3	-2.98	1.32	1.38
1	C	21	TPN	C8'-N1	2.97	1.50	1.46
1	A	17	TPN	C2-N3	-2.88	1.32	1.38
1	A	16	CPN	C4-N3	-2.85	1.29	1.34
1	C	22	CPN	C8'-C7'	2.80	1.57	1.53
1	A	3	CPN	C8'-N1	2.78	1.49	1.46
1	A	5	IPN	C8'-N1	2.76	1.49	1.46
1	C	20	TPN	C8'-N1	2.76	1.49	1.46
1	A	17	TPN	C4-N3	-2.73	1.33	1.38
1	A	20	TPN	C8'-N1	2.72	1.49	1.46
1	C	18	TPN	C8'-N1	2.72	1.49	1.46
1	C	16	CPN	C4-N4	-2.70	1.27	1.33
1	A	1	CPN	C2-N1	-2.70	1.36	1.40
1	A	1	CPN	C8'-C7'	2.64	1.56	1.53
1	A	19	CPN	C4-N3	-2.64	1.29	1.34
1	A	1	CPN	C8'-N1	2.63	1.49	1.46
1	C	16	CPN	C8'-N1	2.60	1.49	1.46
1	A	5	IPN	C2-N3	-2.59	1.33	1.38
1	C	1	CPN	C4-N4	-2.57	1.27	1.33
1	C	17	TPN	C2-N3	-2.56	1.33	1.38
1	A	16	CPN	C4-N4	-2.55	1.27	1.33
1	C	7	TPN	C8'-N1	2.53	1.49	1.46
1	A	19	CPN	C8'-N1	2.50	1.49	1.46
1	C	19	CPN	C8'-N1	2.50	1.49	1.46
1	C	1	CPN	C4-N3	-2.49	1.29	1.34
1	C	22	CPN	C4-N3	-2.49	1.29	1.34
1	A	17	TPN	C8'-N1	2.48	1.49	1.46
1	C	6	CPN	C2-N1	-2.47	1.37	1.40
1	A	23	TPN	C4-N3	-2.47	1.34	1.38
1	C	9	CPN	C4-N4	-2.46	1.28	1.33
1	C	23	TPN	C4-N3	-2.46	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	TPN	C4-N3	-2.45	1.34	1.38
1	C	21	TPN	C2-N3	-2.42	1.33	1.38
1	C	23	TPN	C8'-C7'	2.42	1.56	1.53
1	A	8	TPN	C4-N3	-2.41	1.34	1.38
1	A	21	TPN	C2-N3	-2.38	1.33	1.38
1	C	6	CPN	C8'-C7'	2.37	1.56	1.53
1	A	24	CPN	C8'-N1	2.34	1.49	1.46
1	C	3	CPN	C8'-N1	2.34	1.49	1.46
1	C	7	TPN	C2-N3	-2.32	1.33	1.38
1	C	23	TPN	C8'-N1	2.32	1.49	1.46
1	A	6	CPN	C8'-N1	2.32	1.49	1.46
1	C	1	CPN	C8'-N1	2.31	1.49	1.46
1	C	19	CPN	C4-N4	-2.31	1.28	1.33
1	C	7	TPN	C8'-C7'	2.29	1.56	1.53
1	C	20	TPN	C4-N3	-2.27	1.34	1.38
1	A	23	TPN	C8'-N1	2.24	1.49	1.46
1	C	17	TPN	C4-N3	-2.24	1.34	1.38
1	C	6	CPN	C4-N4	-2.23	1.28	1.33
1	C	4	TPN	C8'-N1	2.22	1.49	1.46
1	C	18	TPN	C8'-C7'	2.21	1.56	1.53
1	A	6	CPN	C4-N4	-2.20	1.28	1.33
1	A	7	TPN	C5'-C	2.19	1.56	1.49
1	A	4	TPN	C8'-N1	2.19	1.49	1.46
1	C	6	CPN	C4-N3	-2.19	1.30	1.34
1	A	24	CPN	C4-N3	-2.19	1.30	1.34
1	A	22	CPN	C4-N3	-2.18	1.30	1.34
1	A	9	CPN	C4-N4	-2.17	1.28	1.33
1	A	18	TPN	C2-N3	-2.17	1.34	1.38
1	A	9	CPN	C4-N3	-2.14	1.30	1.34
1	C	3	CPN	C4-N3	-2.14	1.30	1.34
1	A	24	CPN	C8'-C7'	2.12	1.56	1.53
1	C	2	TPN	C2-N3	-2.12	1.34	1.38
1	A	4	TPN	C2-N3	-2.11	1.34	1.38
1	A	22	CPN	C8'-C7'	2.08	1.56	1.53
1	C	16	CPN	C4-N3	-2.07	1.30	1.34
1	C	1	CPN	C5'-C	2.06	1.56	1.49
1	A	2	TPN	C2-N3	-2.05	1.34	1.38
1	A	20	TPN	C4-N3	-2.04	1.35	1.38
1	A	6	CPN	C4-N3	-2.03	1.30	1.34
1	C	7	TPN	C4-N3	-2.02	1.35	1.38
1	C	24	CPN	C2-N1	-2.02	1.37	1.40
1	A	2	TPN	C8'-N1	2.01	1.48	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	CPN	C4-N4	-2.00	1.29	1.33

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	9	CPN	C7'-C8'-N1	7.60	117.71	110.99
1	A	24	CPN	C-C5'-N4'	-6.73	105.81	113.05
1	A	16	CPN	C7'-C8'-N1	6.29	116.55	110.99
1	A	1	CPN	C8'-C7'-N4'	5.53	124.05	117.08
1	A	23	TPN	C7'-C8'-N1	-5.21	106.39	110.99
1	A	22	CPN	C7'-C8'-N1	-4.97	106.61	110.99
1	C	5	IPN	C4-C5-I5	4.76	126.42	118.54
1	C	3	CPN	N1-C2-N3	4.57	123.07	118.45
1	C	23	TPN	C7'-C8'-N1	-4.41	107.10	110.99
1	A	24	CPN	C7'-C8'-N1	-4.40	107.11	110.99
1	C	22	CPN	C8'-C7'-N4'	4.38	122.60	117.08
1	A	17	TPN	C8'-C7'-N4'	4.35	122.56	117.08
1	A	5	IPN	O4-C4-N3	-4.34	111.79	120.12
1	A	7	TPN	C5M-C5-C4	4.32	123.53	118.77
1	C	5	IPN	O4-C4-N3	-4.29	111.90	120.12
1	A	6	CPN	C8'-C7'-N4'	4.27	122.46	117.08
1	A	1	CPN	C7'-C8'-N1	-4.25	107.24	110.99
1	C	7	TPN	C5M-C5-C4	4.15	123.34	118.77
1	C	17	TPN	C7'-C8'-N1	-4.11	107.36	110.99
1	C	8	TPN	C5M-C5-C4	4.05	123.22	118.77
1	C	6	CPN	C8'-C7'-N4'	3.98	122.10	117.08
1	C	17	TPN	C8'-C7'-N4'	3.96	122.07	117.08
1	A	5	IPN	N3-C2-N1	3.95	118.47	114.86
1	C	20	TPN	C5M-C5-C6	-3.88	117.67	122.85
1	A	21	TPN	C7'-C8'-N1	-3.87	107.57	110.99
1	C	22	CPN	C7'-C8'-N1	-3.87	107.58	110.99
1	A	17	TPN	C5-C6-N1	-3.86	118.98	123.50
1	A	8	TPN	C5M-C5-C4	3.81	122.96	118.77
1	A	20	TPN	C5M-C5-C4	3.80	122.95	118.77
1	A	20	TPN	C5M-C5-C6	-3.80	117.78	122.85
1	A	17	TPN	C7'-C8'-N1	-3.77	107.66	110.99
1	A	20	TPN	C7'-C8'-N1	-3.75	107.68	110.99
1	A	5	IPN	C7'-C8'-N1	3.74	114.30	110.99
1	A	5	IPN	C8'-N1-C6	3.74	124.47	120.08
1	C	8	TPN	C5M-C5-C6	-3.73	117.87	122.85
1	C	21	TPN	C7'-C8'-N1	-3.68	107.75	110.99
1	C	7	TPN	C5M-C5-C6	-3.67	117.94	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	TPN	C7'-C8'-N1	-3.66	107.76	110.99
1	A	22	CPN	C8'-C7'-N4'	3.65	121.69	117.08
1	C	20	TPN	C5M-C5-C4	3.65	122.79	118.77
1	A	19	CPN	C5-C6-N1	-3.65	119.02	122.44
1	A	20	TPN	C8'-C7'-N4'	3.65	121.68	117.08
1	C	21	TPN	C8'-C7'-N4'	3.64	121.67	117.08
1	A	7	TPN	C5M-C5-C6	-3.63	118.00	122.85
1	C	1	CPN	C8'-C7'-N4'	3.61	121.63	117.08
1	C	4	TPN	O2-C2-N1	-3.57	119.72	122.85
1	A	8	TPN	C5M-C5-C6	-3.56	118.09	122.85
1	C	24	CPN	C7'-C8'-N1	-3.56	107.85	110.99
1	C	5	IPN	N3-C2-N1	3.53	118.09	114.86
1	A	8	TPN	C5-C6-N1	-3.48	119.43	123.50
1	A	9	CPN	N1-C2-N3	3.41	121.90	118.45
1	A	2	TPN	C5-C6-N1	-3.41	119.51	123.50
1	A	6	CPN	N1-C2-N3	3.39	121.88	118.45
1	A	18	TPN	C7'-C8'-N1	-3.38	108.00	110.99
1	C	6	CPN	N1-C2-N3	3.37	121.86	118.45
1	C	24	CPN	C5-C6-N1	-3.36	119.29	122.44
1	C	1	CPN	C5-C6-N1	-3.36	119.29	122.44
1	A	7	TPN	O2-C2-N1	-3.36	119.90	122.85
1	C	8	TPN	C5-C6-N1	-3.32	119.61	123.50
1	C	23	TPN	O4-C4-C5	3.32	128.75	124.90
1	C	4	TPN	C8'-C7'-N4'	3.31	121.26	117.08
1	A	3	CPN	N1-C2-N3	3.31	121.80	118.45
1	C	3	CPN	C5-C6-N1	-3.31	119.34	122.44
1	A	3	CPN	C5-C6-N1	-3.29	119.36	122.44
1	A	1	CPN	O7'-C7'-N4'	-3.29	115.64	122.05
1	C	20	TPN	C8'-C7'-N4'	3.26	121.19	117.08
1	C	20	TPN	C7'-C8'-N1	-3.26	108.12	110.99
1	C	21	TPN	C5-C4-N3	3.23	118.07	115.31
1	A	4	TPN	C8'-C7'-N4'	3.17	121.08	117.08
1	C	9	CPN	C5-C6-N1	-3.17	119.48	122.44
1	A	18	TPN	C8'-C7'-N4'	3.15	121.05	117.08
1	A	18	TPN	N3-C2-N1	3.15	117.74	114.86
1	A	21	TPN	C8'-C7'-N4'	3.15	121.05	117.08
1	A	5	IPN	C5-C4-N3	3.14	119.10	113.86
1	A	6	CPN	C5-C6-N1	-3.13	119.51	122.44
1	A	1	CPN	N1-C2-N3	3.13	121.61	118.45
1	C	7	TPN	O2-C2-N1	-3.13	120.10	122.85
1	C	24	CPN	C8'-C7'-N4'	3.13	121.02	117.08
1	A	3	CPN	O-C-C5'	-3.13	116.95	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	CPN	O2-C2-N3	-3.11	117.27	122.33
1	A	23	TPN	C5M-C5-C6	-3.09	118.72	122.85
1	A	2	TPN	C5M-C5-C6	-3.07	118.74	122.85
1	C	4	TPN	N3-C2-N1	3.07	117.66	114.86
1	C	16	CPN	C8'-C7'-N4'	3.06	120.94	117.08
1	C	9	CPN	C5-C4-N3	3.04	126.50	121.33
1	A	18	TPN	C5-C6-N1	-3.04	119.94	123.50
1	A	4	TPN	N3-C2-N1	3.04	117.64	114.86
1	C	2	TPN	C5-C6-N1	-3.02	119.97	123.50
1	A	16	CPN	C2'-C3'-N4'	3.01	118.81	113.11
1	A	16	CPN	C3'-C2'-N	-3.01	102.81	112.69
1	C	5	IPN	C5-C4-N3	2.99	118.84	113.86
1	A	16	CPN	N4-C4-N3	-2.97	112.75	117.97
1	C	2	TPN	C5M-C5-C6	-2.95	118.91	122.85
1	C	1	CPN	O7'-C7'-N4'	-2.95	116.31	122.05
1	A	16	CPN	O-C-C5'	-2.94	117.53	126.39
1	A	4	TPN	C5M-C5-C6	-2.93	118.93	122.85
1	A	4	TPN	C5-C6-N1	-2.92	120.08	123.50
1	C	23	TPN	C5M-C5-C6	-2.91	118.96	122.85
1	A	5	IPN	C8'-N1-C2	-2.91	114.43	117.84
1	C	7	TPN	C5-C6-N1	-2.91	120.09	123.50
1	A	3	CPN	C8'-C7'-N4'	2.91	120.75	117.08
1	A	17	TPN	C5M-C5-C6	-2.91	118.97	122.85
1	C	24	CPN	N4-C4-N3	-2.90	112.89	117.97
1	C	3	CPN	C8'-C7'-N4'	2.89	120.73	117.08
1	A	6	CPN	C8'-N1-C6	2.89	123.92	119.71
1	C	5	IPN	C8'-N1-C6	2.86	123.44	120.08
1	A	16	CPN	C5'-N4'-C3'	-2.86	113.00	117.06
1	C	6	CPN	C5-C6-N1	-2.86	119.77	122.44
1	A	16	CPN	C5-C4-N3	2.84	126.17	121.33
1	C	18	TPN	C5-C6-N1	-2.83	120.19	123.50
1	C	3	CPN	O-C-C5'	-2.83	117.86	126.39
1	A	23	TPN	O4-C4-C5	2.82	128.18	124.90
1	A	23	TPN	C5M-C5-C4	2.82	121.87	118.77
1	C	23	TPN	C5M-C5-C4	2.82	121.87	118.77
1	A	19	CPN	C8'-C7'-N4'	2.81	120.63	117.08
1	A	2	TPN	C5M-C5-C4	2.81	121.86	118.77
1	C	1	CPN	C5-C4-N3	2.81	126.10	121.33
1	C	6	CPN	C8'-N1-C6	2.80	123.79	119.71
1	C	3	CPN	N4-C4-N3	-2.80	113.05	117.97
1	A	21	TPN	C5-C4-N3	2.80	117.70	115.31
1	C	2	TPN	N3-C2-N1	2.79	117.41	114.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	CPN	C5'-N4'-C3'	-2.78	113.11	117.06
1	A	21	TPN	O-C-C5'	-2.78	118.01	126.39
1	A	2	TPN	N3-C2-N1	2.77	117.39	114.86
1	C	17	TPN	C5-C6-N1	-2.76	120.27	123.50
1	C	18	TPN	O-C-C5'	-2.75	118.08	126.39
1	A	21	TPN	C5-C6-N1	-2.75	120.28	123.50
1	C	23	TPN	O-C-C5'	-2.74	118.11	126.39
1	A	3	CPN	N4-C4-N3	-2.73	113.18	117.97
1	A	4	TPN	C5M-C5-C4	2.72	121.76	118.77
1	A	9	CPN	C7'-C8'-N1	2.72	113.39	110.99
1	C	19	CPN	C5-C6-N1	-2.72	119.90	122.44
1	C	21	TPN	O7'-C7'-N4'	-2.71	116.77	122.05
1	A	6	CPN	N4-C4-N3	-2.71	113.21	117.97
1	A	5	IPN	O1'-C'-C5'	-2.69	118.27	126.39
1	C	24	CPN	OXT-C-O	-2.67	116.64	123.30
1	C	22	CPN	C5-C6-N1	-2.67	119.94	122.44
1	C	1	CPN	C7'-C8'-N1	-2.66	108.64	110.99
1	C	4	TPN	C5M-C5-C6	-2.66	119.29	122.85
1	C	21	TPN	O-C-C5'	-2.66	118.36	126.39
1	A	23	TPN	O-C-C5'	-2.66	118.36	126.39
1	C	20	TPN	C5-C6-N1	-2.65	120.40	123.50
1	C	1	CPN	O-C-C5'	-2.65	118.40	126.39
1	C	18	TPN	C8'-C7'-N4'	2.65	120.41	117.08
1	C	24	CPN	C-C5'-N4'	-2.64	110.21	113.05
1	C	17	TPN	O2-C2-N1	2.63	125.16	122.85
1	C	1	CPN	O2-C2-N3	-2.63	118.06	122.33
1	A	16	CPN	C5-C6-N1	-2.63	119.98	122.44
1	C	4	TPN	C5M-C5-C4	2.61	121.64	118.77
1	C	24	CPN	C8'-N1-C6	2.61	123.50	119.71
1	A	18	TPN	O4-C4-N3	-2.60	115.13	120.12
1	C	17	TPN	C5M-C5-C6	-2.59	119.39	122.85
1	C	16	CPN	O-C-C5'	-2.59	118.57	126.39
1	C	4	TPN	C7'-C8'-N1	-2.59	108.71	110.99
1	C	4	TPN	C5-C6-N1	-2.59	120.47	123.50
1	A	24	CPN	C8'-C7'-N4'	2.58	120.34	117.08
1	C	21	TPN	C5-C6-N1	-2.58	120.48	123.50
1	A	18	TPN	O-C-C5'	-2.57	118.63	126.39
1	A	1	CPN	N4-C4-N3	-2.57	113.46	117.97
1	C	24	CPN	N1-C2-N3	2.56	121.04	118.45
1	A	9	CPN	C5-C4-N3	2.56	125.69	121.33
1	A	17	TPN	C5M-C5-C4	2.56	121.59	118.77
1	A	19	CPN	N4-C4-N3	-2.56	113.47	117.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	CPN	O2-C2-N3	-2.55	118.19	122.33
1	A	17	TPN	O-C-C5'	-2.55	118.70	126.39
1	C	22	CPN	O-C-C5'	-2.54	118.71	126.39
1	A	23	TPN	C5-C6-N1	-2.54	120.53	123.50
1	C	23	TPN	C8'-C7'-N4'	2.53	120.27	117.08
1	C	9	CPN	C5'-N4'-C3'	-2.52	113.48	117.06
1	C	5	IPN	C7'-C8'-N1	2.52	113.22	110.99
1	A	24	CPN	OXT-C-O	-2.52	117.02	123.30
1	C	17	TPN	C3'-C2'-N	-2.52	104.42	112.69
1	C	18	TPN	N3-C2-N1	2.51	117.16	114.86
1	C	23	TPN	C5-C6-N1	-2.51	120.56	123.50
1	A	20	TPN	C5-C6-N1	-2.50	120.57	123.50
1	C	17	TPN	O-C-C5'	-2.49	118.86	126.39
1	C	21	TPN	C5M-C5-C4	2.49	121.51	118.77
1	A	6	CPN	C5-C4-N3	2.49	125.56	121.33
1	C	19	CPN	C8'-C7'-N4'	2.48	120.20	117.08
1	A	6	CPN	C4-N3-C2	-2.46	116.28	120.25
1	A	2	TPN	O-C-C5'	-2.45	118.98	126.39
1	C	5	IPN	C8'-N1-C2	-2.44	114.99	117.84
1	C	2	TPN	C5M-C5-C4	2.43	121.44	118.77
1	A	1	CPN	O2-C2-N3	-2.43	118.38	122.33
1	C	4	TPN	C8'-N1-C6	2.43	122.93	120.08
1	C	3	CPN	C4-N3-C2	-2.42	116.36	120.25
1	C	7	TPN	O-C-C5'	-2.42	119.10	126.39
1	A	22	CPN	O-C-C5'	-2.41	119.10	126.39
1	A	4	TPN	C8'-N1-C6	2.41	122.91	120.08
1	C	9	CPN	N1-C2-N3	2.40	120.88	118.45
1	C	21	TPN	O4-C4-N3	-2.40	115.52	120.12
1	A	9	CPN	C4-N3-C2	-2.40	116.38	120.25
1	C	9	CPN	C4-N3-C2	-2.39	116.39	120.25
1	A	5	IPN	C4-N3-C2	-2.39	124.26	127.35
1	A	17	TPN	N3-C2-N1	2.38	117.03	114.86
1	C	16	CPN	C5-C4-N3	2.38	125.37	121.33
1	A	4	TPN	O2-C2-N1	-2.38	120.77	122.85
1	C	19	CPN	O-C-C5'	-2.37	119.22	126.39
1	C	1	CPN	N4-C4-N3	-2.37	113.80	117.97
1	A	23	TPN	C8'-C7'-N4'	2.37	120.07	117.08
1	A	4	TPN	C8'-N1-C2	-2.37	115.06	117.84
1	C	5	IPN	C4-N3-C2	-2.37	124.29	127.35
1	C	1	CPN	C2'-C3'-N4'	-2.36	108.65	113.11
1	C	6	CPN	O-C-C5'	-2.35	119.28	126.39
1	A	5	IPN	C8'-C7'-N4'	2.35	120.04	117.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	CPN	O-C-C5'	-2.34	119.33	126.39
1	A	18	TPN	C5-C4-N3	2.34	117.31	115.31
1	A	19	CPN	C5-C4-N3	2.33	125.30	121.33
1	A	1	CPN	C5-C4-N3	2.33	125.29	121.33
1	A	22	CPN	C5-C4-N3	2.33	125.29	121.33
1	C	4	TPN	C8'-N1-C2	-2.32	115.13	117.84
1	C	18	TPN	C5-C4-N3	2.31	117.28	115.31
1	C	22	CPN	N4-C4-N3	-2.30	113.92	117.97
1	C	2	TPN	C7'-C8'-N1	2.30	113.03	110.99
1	C	9	CPN	N4-C4-N3	-2.30	113.93	117.97
1	A	22	CPN	N4-C4-N3	-2.30	113.94	117.97
1	A	18	TPN	O4-C4-C5	2.29	127.56	124.90
1	A	3	CPN	C5-C4-N3	2.29	125.22	121.33
1	A	22	CPN	C5-C6-N1	-2.29	120.30	122.44
1	A	9	CPN	O-C-C5'	-2.26	119.57	126.39
1	A	4	TPN	C7'-C8'-N1	-2.25	109.00	110.99
1	C	3	CPN	C7'-C8'-N1	2.25	112.98	110.99
1	C	1	CPN	N1-C2-N3	2.25	120.72	118.45
1	C	17	TPN	N3-C2-N1	2.25	116.91	114.86
1	C	22	CPN	O7'-C7'-N4'	-2.24	117.68	122.05
1	C	24	CPN	C5-C4-N3	2.24	125.14	121.33
1	C	19	CPN	N4-C4-N3	-2.24	114.04	117.97
1	C	16	CPN	O7'-C7'-C8'	-2.23	117.11	120.59
1	C	2	TPN	O-C-C5'	-2.22	119.67	126.39
1	C	3	CPN	C5-C4-N3	2.22	125.10	121.33
1	C	19	CPN	C5-C4-N3	2.22	125.10	121.33
1	C	9	CPN	C8'-N1-C6	2.21	122.92	119.71
1	C	8	TPN	O-C-C5'	-2.20	119.74	126.39
1	A	3	CPN	C8'-N1-C6	2.20	122.91	119.71
1	C	18	TPN	O4-C4-N3	-2.20	115.90	120.12
1	C	3	CPN	C8'-N1-C6	2.20	122.91	119.71
1	C	17	TPN	C5M-C5-C4	2.19	121.18	118.77
1	A	21	TPN	O4-C4-N3	-2.17	115.95	120.12
1	A	20	TPN	O7'-C7'-N4'	-2.17	117.82	122.05
1	A	2	TPN	C5-C4-N3	2.16	117.16	115.31
1	A	21	TPN	C5M-C5-C4	2.16	121.14	118.77
1	C	1	CPN	C4-N3-C2	-2.16	116.77	120.25
1	C	22	CPN	C5-C4-N3	2.16	124.99	121.33
1	C	6	CPN	C3'-C2'-N	2.15	119.76	112.69
1	C	2	TPN	C8'-C7'-N4'	2.14	119.78	117.08
1	A	7	TPN	C5-C6-N1	-2.14	120.99	123.50
1	A	9	CPN	O2-C2-N3	-2.13	118.86	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	9	CPN	C8'-C7'-N4'	2.12	119.75	117.08
1	A	18	TPN	O7'-C7'-N4'	-2.11	117.93	122.05
1	C	21	TPN	N3-C2-N1	2.11	116.79	114.86
1	A	22	CPN	O7'-C7'-N4'	-2.11	117.93	122.05
1	A	3	CPN	C4-N3-C2	-2.11	116.85	120.25
1	A	3	CPN	C7'-C8'-N1	2.10	112.85	110.99
1	A	6	CPN	O-C-C5'	-2.09	120.06	126.39
1	C	20	TPN	O7'-C7'-N4'	-2.09	117.97	122.05
1	A	8	TPN	O-C-C5'	-2.09	120.08	126.39
1	A	20	TPN	O-C-C5'	-2.09	120.08	126.39
1	C	5	IPN	O1'-C'-C5'	-2.06	120.16	126.39
1	C	17	TPN	O7'-C7'-N4'	-2.05	118.05	122.05
1	A	5	IPN	C5'-N4'-C3'	2.05	119.97	117.06
1	C	7	TPN	C8'-C7'-N4'	2.04	119.66	117.08
1	C	9	CPN	O2-C2-N1	-2.04	117.10	119.24
1	C	21	TPN	C5'-N4'-C3'	2.03	119.94	117.06
1	A	24	CPN	N4-C4-N3	-2.02	114.42	117.97
1	C	5	IPN	O4-C4-C5	2.00	129.26	125.69

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	9	CPN	C-C5'-N4'-C7'
1	A	9	CPN	C-C5'-N4'-C3'
1	A	16	CPN	C-C5'-N4'-C7'
1	A	17	TPN	N-C2'-C3'-N4'
1	C	9	CPN	C-C5'-N4'-C7'
1	C	17	TPN	N-C2'-C3'-N4'
1	A	16	CPN	C-C5'-N4'-C3'
1	A	16	CPN	C7'-C8'-N1-C6
1	A	16	CPN	C7'-C8'-N1-C2
1	C	9	CPN	C-C5'-N4'-C3'

There are no ring outliers.

7 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	1	CPN	1	0
1	C	16	CPN	1	0
1	C	22	CPN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	24	CPN	2	0
1	C	21	TPN	1	0
1	C	24	CPN	1	0
1	A	1	CPN	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	6/24 (25%)	-0.58	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	24, 30, 36, 37	0
1	C	6/24 (25%)	1.29	2 (33%) <span style="border: 1px solid red; padding: 2px;">0</span> <span style="border: 1px solid red; padding: 2px;">0</span>	27, 39, 45, 45	0
2	B	9/9 (100%)	-0.72	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	14, 19, 22, 23	0
2	D	9/9 (100%)	-0.94	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	12, 14, 16, 17	0
All	All	30/66 (45%)	-0.36	2 (6%) <span style="border: 1px solid red; padding: 2px;">17</span> <span style="border: 1px solid red; padding: 2px;">18</span>	12, 21, 43, 45	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	10	HIS	3.1
1	C	13	SER	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	TPN	A	8	19/20	0.91	0.13	0,11,27,28	0
1	TPN	A	7	19/20	0.92	0.17	0,21,27,29	0
1	CPN	A	6	18/19	0.92	0.14	0,14,28,34	0
1	CPN	A	16	18/19	0.92	0.13	0,18,25,33	0
1	CPN	C	3	18/19	0.92	0.15	0,11,27,39	0
1	TPN	C	4	19/20	0.92	0.12	0,12,25,28	0
1	TPN	A	23	19/20	0.93	0.14	0,16,22,26	0
1	TPN	C	2	19/20	0.93	0.13	0,12,24,31	0
1	TPN	C	17	19/20	0.93	0.12	0,15,20,22	0
1	TPN	A	17	19/20	0.94	0.17	0,14,24,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CPN	A	22	18/19	0.94	0.11	0,13,26,27	0
1	TPN	A	2	19/20	0.94	0.15	0,10,18,21	0
1	CPN	C	16	18/19	0.94	0.15	0,19,24,26	0
1	CPN	C	1	18/19	0.94	0.11	0,15,28,33	0
1	TPN	C	18	19/20	0.94	0.10	0,12,21,23	0
1	CPN	C	24	19/19	0.94	0.13	0,13,17,20	0
1	CPN	A	9	18/19	0.95	0.11	0,14,28,29	0
1	CPN	A	24	19/19	0.95	0.10	0,17,28,31	0
1	TPN	A	20	19/20	0.95	0.10	0,16,22,27	0
1	TPN	A	21	19/20	0.95	0.10	0,14,27,31	0
1	CPN	A	3	18/19	0.95	0.12	0,10,16,18	0
1	TPN	C	8	19/20	0.96	0.15	0,10,13,20	0
1	CPN	C	9	18/19	0.96	0.13	0,9,24,34	0
1	CPN	A	19	18/19	0.96	0.10	0,13,21,23	0
1	CPN	A	1	18/19	0.96	0.11	0,7,14,21	0
1	CPN	C	6	18/19	0.96	0.11	0,9,16,21	0
1	TPN	C	23	19/20	0.96	0.10	0,8,15,17	0
1	TPN	C	7	19/20	0.96	0.16	0,9,17,22	0
1	CPN	C	19	18/19	0.97	0.12	0,14,18,19	0
1	TPN	C	20	19/20	0.97	0.10	0,10,15,20	0
1	CPN	C	22	18/19	0.97	0.11	0,12,16,22	0
1	TPN	A	18	19/20	0.97	0.12	0,14,19,20	0
1	TPN	A	4	19/20	0.97	0.10	0,11,17,24	0
1	TPN	C	21	19/20	0.98	0.09	0,11,19,22	0
1	IPN	A	5	19/20	0.99	0.12	0,23,26,27	0
1	IPN	C	5	19/20	0.99	0.11	0,16,24,27	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.