



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 12:38 PM EDT

PDB ID : 3MBS  
Title : Crystal structure of 8mer PNA  
Authors : Yeh, J.I.; Pohl, E.; Truan, D.; He, W.; Sheldrick, G.M.; Achim, C.  
Deposited on : unknown  
Resolution : 1.27 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

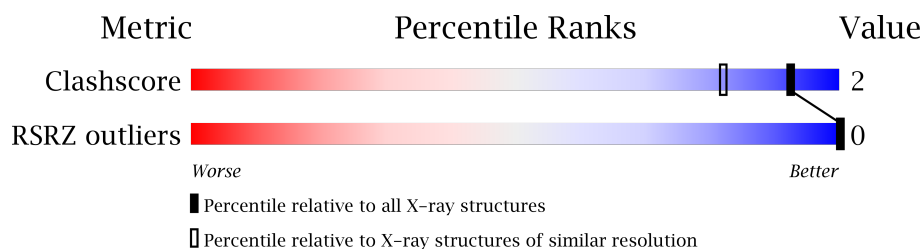
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 1.27 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	112137	1447 (1.30-1.26)
RSRZ outliers	101464	1370 (1.30-1.26)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	9	 89% 11%
1	B	9	 89% 11%
1	C	9	 89% 11%
1	D	9	 78% 11% 11%

## 2 Entry composition [i](#)

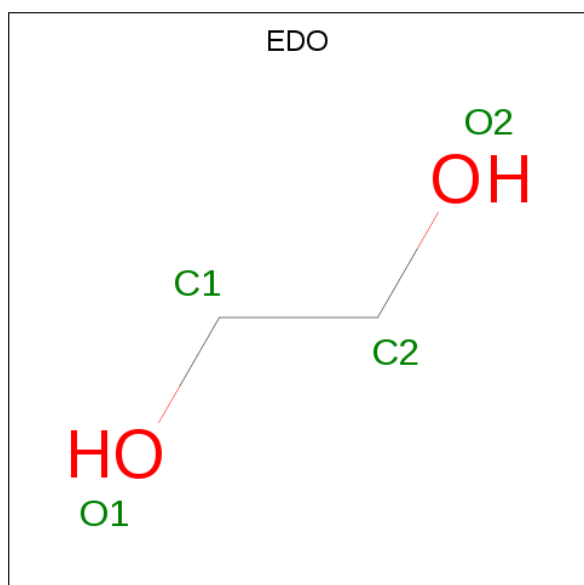
There are 3 unique types of molecules in this entry. The entry contains 892 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DNA chain called Peptide Nucleic Acid.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	9	Total	C	N	O	0	0	1
			157	85	48	24			
1	B	8	Total	C	N	O	0	0	0
			156	85	47	24			
1	C	9	Total	C	N	O	0	0	0
			159	87	48	24			
1	D	8	Total	C	N	O	0	0	0
			152	83	46	23			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	68	Total	O	0	0
			68	68		
3	C	60	Total	O	0	0
			60	60		
3	D	59	Total	O	0	0
			59	59		

### 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: Peptide Nucleic Acid

Chain A:  89% 11%



- Molecule 1: Peptide Nucleic Acid

Chain B:  89% 11%




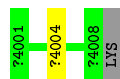
- Molecule 1: Peptide Nucleic Acid

Chain C:  89% 11%



- Molecule 1: Peptide Nucleic Acid

Chain D:  78% 11% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	18.87Å 28.92Å 54.97Å 88.10° 85.75° 79.56°	Depositor
Resolution (Å)	18.51 – 1.27 18.51 – 1.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (18.51-1.27) 82.2 (18.51-1.22)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 1.22Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.179 , 0.220 0.184 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	11.3	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 92.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.59$ , $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	892	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.21% 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: TPN, GPN, APN, EDO, CPN

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	C	7.76	1/2 (50.0%)	7.15	1/1 (100.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3009	LYS	N-CA	-10.84	1.24	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3009	LYS	N-CA-C	7.15	130.32	111.00

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	157	0	107	1	0
1	B	156	0	107	0	0
1	C	159	0	107	0	0
1	D	152	0	98	1	0
2	A	8	0	12	0	0
2	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	8	0	12	0	0
3	A	61	0	0	1	0
3	B	68	0	0	0	0
3	C	60	0	0	0	0
3	D	59	0	0	1	0
All	All	892	0	449	2	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 2.

All (2) 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:1009:LYS:N	3:A:9006:HOH:O	2.48	0.47
1:D:4004:APN:H5'1	3:D:9085:HOH:O	2.21	0.41

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](#)

32 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	GPN	A	1001	1	18,22,23	1.05	1 (5%)	19,30,32	2.86	9 (47%)
1	GPN	A	1002	1	18,22,23	1.24	2 (11%)	19,30,32	2.84	6 (31%)
1	CPN	A	1003	1	15,18,19	0.99	1 (6%)	17,23,25	1.57	4 (23%)
1	APN	A	1004	1	18,21,22	0.90	0	17,28,30	1.53	4 (23%)
1	TPN	A	1005	1	15,19,20	1.22	1 (6%)	18,25,27	3.61	4 (22%)
1	GPN	A	1006	1	18,22,23	1.37	2 (11%)	19,30,32	2.55	10 (52%)
1	CPN	A	1007	1	15,18,19	1.06	2 (13%)	17,23,25	1.38	2 (11%)
1	CPN	A	1008	1	15,18,19	1.03	1 (6%)	17,23,25	1.54	3 (17%)
1	GPN	B	2001	1	18,22,23	1.21	2 (11%)	19,30,32	2.72	10 (52%)
1	GPN	B	2002	1	18,22,23	1.34	2 (11%)	19,30,32	2.70	9 (47%)
1	CPN	B	2003	1	15,18,19	1.07	1 (6%)	17,23,25	1.09	2 (11%)
1	APN	B	2004	1	18,21,22	0.94	1 (5%)	17,28,30	2.02	5 (29%)
1	TPN	B	2005	1	15,19,20	1.16	1 (6%)	18,25,27	3.53	4 (22%)
1	GPN	B	2006	1	18,22,23	1.42	1 (5%)	19,30,32	2.62	6 (31%)
1	CPN	B	2007	1	15,18,19	0.85	1 (6%)	17,23,25	1.18	2 (11%)
1	CPN	B	2008	1	15,18,19	1.14	2 (13%)	17,23,25	0.85	0
1	GPN	C	3001	1	18,22,23	1.24	2 (11%)	19,30,32	2.81	7 (36%)
1	GPN	C	3002	1	18,22,23	1.19	2 (11%)	19,30,32	2.44	6 (31%)
1	CPN	C	3003	1	15,18,19	1.03	1 (6%)	17,23,25	1.53	3 (17%)
1	APN	C	3004	1	18,21,22	0.74	0	17,28,30	1.91	4 (23%)
1	TPN	C	3005	1	15,19,20	0.95	1 (6%)	18,25,27	3.19	6 (33%)
1	GPN	C	3006	1	18,22,23	1.15	1 (5%)	19,30,32	2.77	5 (26%)
1	CPN	C	3007	1	15,18,19	1.09	2 (13%)	17,23,25	1.66	5 (29%)
1	CPN	C	3008	1	15,18,19	1.44	3 (20%)	17,23,25	1.75	4 (23%)
1	GPN	D	4001	1	16,20,23	1.19	1 (6%)	18,28,32	2.85	6 (33%)
1	GPN	D	4002	1	18,22,23	1.35	2 (11%)	19,30,32	2.57	5 (26%)
1	CPN	D	4003	1	15,18,19	1.10	2 (13%)	17,23,25	1.25	1 (5%)
1	APN	D	4004	1	18,21,22	0.82	0	17,28,30	1.95	6 (35%)
1	TPN	D	4005	1	15,19,20	1.40	2 (13%)	18,25,27	4.00	7 (38%)
1	GPN	D	4006	1	18,22,23	1.24	2 (11%)	19,30,32	3.31	10 (52%)
1	CPN	D	4007	1	15,18,19	1.06	2 (13%)	17,23,25	1.09	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CPN	D	4008	1	13,16,19	1.04	1 (7%)	15,21,25	0.99	1 (6%)

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
1	GPN	A	1001	1	-	0/13/14/15	0/2/2/2
1	GPN	A	1002	1	-	0/13/14/15	0/2/2/2
1	CPN	A	1003	1	-	0/13/14/15	0/1/1/1
1	APN	A	1004	1	-	0/13/14/15	0/2/2/2
1	TPN	A	1005	1	-	0/13/14/15	0/1/1/1
1	GPN	A	1006	1	-	0/13/14/15	0/2/2/2
1	CPN	A	1007	1	-	0/13/14/15	0/1/1/1
1	CPN	A	1008	1	-	0/13/14/15	0/1/1/1
1	GPN	B	2001	1	-	0/13/14/15	0/2/2/2
1	GPN	B	2002	1	-	0/13/14/15	0/2/2/2
1	CPN	B	2003	1	-	0/13/14/15	0/1/1/1
1	APN	B	2004	1	-	0/13/14/15	0/2/2/2
1	TPN	B	2005	1	-	0/13/14/15	0/1/1/1
1	GPN	B	2006	1	-	0/13/14/15	0/2/2/2
1	CPN	B	2007	1	-	0/13/14/15	0/1/1/1
1	CPN	B	2008	1	-	0/13/14/15	0/1/1/1
1	GPN	C	3001	1	-	0/13/14/15	0/2/2/2
1	GPN	C	3002	1	-	0/13/14/15	0/2/2/2
1	CPN	C	3003	1	-	0/13/14/15	0/1/1/1
1	APN	C	3004	1	-	0/13/14/15	0/2/2/2
1	TPN	C	3005	1	-	0/13/14/15	0/1/1/1
1	GPN	C	3006	1	-	0/13/14/15	0/2/2/2
1	CPN	C	3007	1	-	0/13/14/15	0/1/1/1
1	CPN	C	3008	1	-	0/13/14/15	0/1/1/1
1	GPN	D	4001	1	-	0/10/11/15	0/2/2/2
1	GPN	D	4002	1	-	0/13/14/15	0/2/2/2
1	CPN	D	4003	1	-	0/13/14/15	0/1/1/1
1	APN	D	4004	1	-	0/13/14/15	0/2/2/2
1	TPN	D	4005	1	-	0/13/14/15	0/1/1/1
1	GPN	D	4006	1	-	0/13/14/15	0/2/2/2
1	CPN	D	4007	1	-	0/13/14/15	0/1/1/1
1	CPN	D	4008	1	-	0/11/11/15	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3007	CPN	C8'-N1	-2.98	1.44	1.47
1	B	2008	CPN	C8'-N1	-2.73	1.44	1.47
1	B	2007	CPN	C8'-N1	-2.23	1.45	1.47
1	D	4006	GPN	C6-C5	-2.23	1.37	1.41
1	C	3008	CPN	C8'-N1	-2.04	1.45	1.47
1	C	3005	TPN	C4-N3	2.00	1.36	1.33
1	D	4005	TPN	C6-N1	2.02	1.41	1.36
1	D	4007	CPN	C4-N3	2.09	1.39	1.35
1	D	4003	CPN	C6-N1	2.11	1.39	1.36
1	D	4002	GPN	C2-N1	2.13	1.39	1.35
1	A	1007	CPN	C6-N1	2.15	1.39	1.36
1	C	3007	CPN	C6-N1	2.23	1.39	1.36
1	C	3002	GPN	C2-N1	2.26	1.39	1.35
1	A	1003	CPN	C4-N3	2.26	1.39	1.35
1	A	1007	CPN	C4-N3	2.28	1.39	1.35
1	C	3001	GPN	C2-N1	2.31	1.39	1.35
1	C	3003	CPN	C4-N3	2.36	1.39	1.35
1	B	2002	GPN	C2-N1	2.41	1.39	1.35
1	D	4007	CPN	C6-N1	2.46	1.40	1.36
1	B	2008	CPN	C4-N3	2.52	1.39	1.35
1	D	4003	CPN	C4-N3	2.57	1.39	1.35
1	A	1008	CPN	C6-N1	2.60	1.40	1.36
1	B	2001	GPN	C2-N1	2.67	1.40	1.35
1	D	4008	CPN	C4-N3	2.67	1.40	1.35
1	C	3008	CPN	C4-N3	2.83	1.40	1.35
1	B	2003	CPN	C6-N1	2.85	1.40	1.36
1	A	1002	GPN	C2-N1	2.86	1.40	1.35
1	B	2004	APN	C5'-N4'	2.88	1.52	1.47
1	C	3002	GPN	C6-N1	3.02	1.38	1.33
1	A	1001	GPN	C6-N1	3.03	1.38	1.33
1	A	1006	GPN	C2-N1	3.27	1.41	1.35
1	A	1002	GPN	C6-N1	3.44	1.39	1.33
1	B	2001	GPN	C6-N1	3.56	1.39	1.33
1	B	2005	TPN	C4-N3	3.59	1.39	1.33
1	D	4006	GPN	C6-N1	3.63	1.39	1.33
1	C	3001	GPN	C6-N1	3.79	1.39	1.33
1	C	3006	GPN	C6-N1	3.91	1.40	1.33
1	C	3008	CPN	C6-N1	3.92	1.42	1.36
1	A	1005	TPN	C4-N3	3.94	1.40	1.33
1	D	4001	GPN	C6-N1	3.99	1.40	1.33
1	A	1006	GPN	C6-N1	4.00	1.40	1.33
1	D	4002	GPN	C6-N1	4.05	1.40	1.33
1	B	2002	GPN	C6-N1	4.15	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4005	TPN	C4-N3	4.19	1.40	1.33
1	B	2006	GPN	C6-N1	5.52	1.43	1.33

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3006	GPN	C5-C6-N1	-8.01	112.07	123.48
1	A	1001	GPN	C5-C6-N1	-7.50	112.81	123.48
1	D	4001	GPN	C5-C6-N1	-7.47	112.84	123.48
1	D	4002	GPN	C5-C6-N1	-7.19	113.25	123.48
1	A	1005	TPN	C5-C4-N3	-7.16	117.34	125.24
1	A	1002	GPN	C5-C6-N1	-7.05	113.44	123.48
1	B	2005	TPN	C5-C4-N3	-7.03	117.48	125.24
1	D	4006	GPN	C5-C6-N1	-6.95	113.58	123.48
1	D	4005	TPN	C5-C4-N3	-6.87	117.67	125.24
1	B	2006	GPN	C5-C6-N1	-6.67	113.98	123.48
1	C	3002	GPN	C5-C6-N1	-6.14	114.74	123.48
1	B	2002	GPN	C5-C6-N1	-6.10	114.80	123.48
1	C	3001	GPN	C5-C6-N1	-6.10	114.80	123.48
1	D	4006	GPN	N3-C2-N1	-5.88	118.87	127.46
1	B	2001	GPN	N3-C2-N1	-5.80	118.99	127.46
1	C	3005	TPN	C5-C4-N3	-5.26	119.44	125.24
1	D	4006	GPN	C7'-C8'-N9	-5.24	104.52	110.79
1	C	3001	GPN	C7'-C8'-N9	-5.06	104.74	110.79
1	B	2002	GPN	N3-C2-N1	-4.90	120.30	127.46
1	A	1002	GPN	N3-C2-N1	-4.90	120.30	127.46
1	B	2001	GPN	C5-C6-N1	-4.88	116.54	123.48
1	C	3001	GPN	N3-C2-N1	-4.74	120.54	127.46
1	B	2006	GPN	C7'-C8'-N9	-4.69	105.19	110.79
1	C	3006	GPN	C7'-C8'-N9	-4.68	105.19	110.79
1	C	3004	APN	N3-C2-N1	-4.64	124.81	128.86
1	A	1006	GPN	C5-C6-N1	-4.61	116.92	123.48
1	C	3008	CPN	C5-C6-N1	-4.40	117.60	121.35
1	D	4004	APN	N3-C2-N1	-4.29	125.12	128.86
1	C	3002	GPN	N3-C2-N1	-4.18	121.36	127.46
1	B	2004	APN	N3-C2-N1	-4.03	125.35	128.86
1	C	3005	TPN	C'-C5'-N4'	-3.86	105.24	112.91
1	D	4001	GPN	N3-C2-N1	-3.81	121.90	127.46
1	B	2002	GPN	C4-C5-N7	-3.76	105.78	109.41
1	A	1003	CPN	C5-C6-N1	-3.69	118.20	121.35
1	B	2006	GPN	N3-C2-N1	-3.64	122.14	127.46
1	C	3006	GPN	N3-C2-N1	-3.64	122.14	127.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4002	GPN	N3-C2-N1	-3.57	122.25	127.46
1	A	1006	GPN	N3-C2-N1	-3.51	122.33	127.46
1	A	1005	TPN	C'-C5'-N4'	-3.43	106.09	112.91
1	D	4001	GPN	O1'-C'-C5'	-3.40	115.14	126.38
1	A	1001	GPN	C7'-C8'-N9	-3.34	106.79	110.79
1	D	4001	GPN	C7'-C8'-N9	-3.27	106.88	110.79
1	B	2001	GPN	C7'-C8'-N9	-3.23	106.92	110.79
1	A	1006	GPN	N2-C2-N1	-3.18	112.15	117.24
1	D	4003	CPN	O1'-C'-C5'	-3.16	115.92	126.38
1	B	2004	APN	C4-C5-N7	-3.15	106.37	109.41
1	A	1001	GPN	N3-C2-N1	-3.13	122.88	127.46
1	A	1002	GPN	O1'-C'-C5'	-3.09	116.18	126.38
1	A	1002	GPN	C6-C5-C4	-3.06	117.80	120.84
1	B	2004	APN	C8'-N9-C8	-3.06	122.03	125.67
1	D	4004	APN	O1'-C'-C5'	-2.95	116.61	126.38
1	C	3002	GPN	C4-C5-N7	-2.95	106.56	109.41
1	D	4004	APN	C5'-N4'-C7'	-2.94	112.44	120.84
1	A	1008	CPN	O1'-C'-C5'	-2.86	116.93	126.38
1	C	3004	APN	O1'-C'-C5'	-2.86	116.94	126.38
1	C	3001	GPN	O1'-C'-C5'	-2.76	117.26	126.38
1	C	3002	GPN	O1'-C'-C5'	-2.73	117.34	126.38
1	A	1003	CPN	C5'-N4'-C7'	-2.71	113.09	120.84
1	C	3008	CPN	C'-C5'-N4'	-2.71	107.54	112.91
1	A	1006	GPN	C7'-C8'-N9	-2.70	107.56	110.79
1	B	2007	CPN	O1'-C'-C5'	-2.70	117.47	126.38
1	A	1007	CPN	O1'-C'-C5'	-2.63	117.68	126.38
1	A	1003	CPN	O1'-C'-C5'	-2.62	117.72	126.38
1	D	4006	GPN	C4-C5-N7	-2.62	106.88	109.41
1	A	1006	GPN	O1'-C'-C5'	-2.59	117.82	126.38
1	A	1004	APN	N3-C2-N1	-2.58	126.61	128.86
1	D	4002	GPN	O1'-C'-C5'	-2.58	117.86	126.38
1	D	4006	GPN	C5'-N4'-C7'	-2.56	113.52	120.84
1	B	2004	APN	C7'-C8'-N9	-2.56	107.73	110.79
1	B	2001	GPN	C6-C5-C4	-2.55	118.31	120.84
1	A	1006	GPN	O7'-C7'-C8'	-2.54	116.55	120.63
1	B	2002	GPN	O1'-C'-C5'	-2.51	118.09	126.38
1	C	3005	TPN	O7'-C7'-N4'	-2.48	117.10	122.05
1	C	3001	GPN	C4-C5-N7	-2.48	107.02	109.41
1	C	3003	CPN	O1'-C'-C5'	-2.47	118.20	126.38
1	A	1008	CPN	C5-C6-N1	-2.46	119.25	121.35
1	B	2001	GPN	O1'-C'-C5'	-2.43	118.36	126.38
1	D	4006	GPN	O7'-C7'-N4'	-2.41	117.25	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3007	CPN	O1'-C'-C5'	-2.31	118.76	126.38
1	B	2006	GPN	O1'-C'-C5'	-2.29	118.81	126.38
1	D	4006	GPN	C8'-N9-C8	-2.29	122.95	125.67
1	A	1005	TPN	C5'-N4'-C7'	-2.28	114.33	120.84
1	D	4007	CPN	O1'-C'-C5'	-2.27	118.86	126.38
1	D	4004	APN	C8'-N9-C8	-2.27	122.97	125.67
1	C	3001	GPN	O7'-C7'-N4'	-2.26	117.54	122.05
1	A	1001	GPN	O1'-C'-C5'	-2.22	119.05	126.38
1	B	2003	CPN	O1'-C'-C5'	-2.19	119.12	126.38
1	A	1004	APN	C4-C5-N7	-2.19	107.30	109.41
1	A	1001	GPN	C2-N3-C4	-2.16	112.64	115.16
1	B	2005	TPN	C'-C5'-N4'	-2.15	108.63	112.91
1	D	4006	GPN	C6-C5-C4	-2.14	118.72	120.84
1	D	4008	CPN	C7'-C8'-N1	-2.13	108.25	110.79
1	D	4005	TPN	C'-C5'-N4'	-2.13	108.69	112.91
1	C	3002	GPN	C6-C5-C4	-2.12	118.74	120.84
1	D	4005	TPN	C5'-N4'-C7'	-2.10	114.85	120.84
1	A	1001	GPN	O7'-C7'-N4'	-2.08	117.90	122.05
1	C	3007	CPN	O7'-C7'-C8'	-2.06	117.31	120.63
1	A	1006	GPN	C4-C5-N7	-2.05	107.43	109.41
1	B	2002	GPN	O7'-C7'-C8'	-2.03	117.37	120.63
1	D	4005	TPN	O1'-C'-C5'	-2.02	119.71	126.38
1	B	2007	CPN	C5-C6-N1	-2.01	119.63	121.35
1	D	4002	GPN	C6-C5-C4	-2.01	118.84	120.84
1	B	2004	APN	C'-C5'-N4'	2.03	116.93	112.91
1	B	2003	CPN	C8'-N1-C6	2.05	122.56	118.72
1	B	2002	GPN	C2-N3-C4	2.12	117.63	115.16
1	B	2006	GPN	C2'-C3'-N4'	2.15	117.34	113.44
1	C	3006	GPN	N2-C2-N3	2.16	121.74	117.75
1	A	1007	CPN	C8'-N1-C6	2.17	122.78	118.72
1	D	4001	GPN	N2-C2-N3	2.17	121.75	117.75
1	C	3007	CPN	C'-C5'-N4'	2.23	117.33	112.91
1	A	1003	CPN	C7'-C8'-N1	2.24	113.46	110.79
1	C	3005	TPN	C8'-C7'-N4'	2.25	120.01	117.05
1	A	1008	CPN	C3'-N4'-C7'	2.29	128.01	120.79
1	C	3008	CPN	C8'-N1-C2	2.29	120.46	117.86
1	A	1002	GPN	N2-C2-N3	2.42	122.22	117.75
1	D	4006	GPN	C8'-C7'-N4'	2.45	120.27	117.05
1	C	3003	CPN	C8'-C7'-N4'	2.46	120.29	117.05
1	C	3008	CPN	C8'-C7'-N4'	2.49	120.32	117.05
1	C	3007	CPN	C8'-N1-C2	2.52	120.72	117.86
1	B	2005	TPN	O7'-C7'-N4'	2.52	127.06	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3007	CPN	C8'-C7'-N4'	2.53	120.38	117.05
1	B	2002	GPN	C2'-C3'-N4'	2.53	118.04	113.44
1	A	1001	GPN	C8'-N9-C8	2.54	128.68	125.67
1	C	3005	TPN	C2'-C3'-N4'	2.55	118.08	113.44
1	C	3004	APN	C8'-N9-C8	2.61	128.76	125.67
1	B	2001	GPN	C8'-C7'-N4'	2.63	120.51	117.05
1	D	4004	APN	C2'-C3'-N4'	2.66	118.28	113.44
1	B	2001	GPN	C8'-N9-C8	2.66	128.83	125.67
1	A	1004	APN	C'-C5'-N4'	2.68	118.22	112.91
1	D	4004	APN	C8'-C7'-N4'	2.69	120.60	117.05
1	A	1004	APN	C8'-N9-C8	2.76	128.95	125.67
1	A	1001	GPN	C8'-C7'-N4'	2.86	120.82	117.05
1	B	2001	GPN	C2-N3-C4	2.87	118.50	115.16
1	A	1006	GPN	C6-N1-C2	2.87	120.19	116.06
1	D	4005	TPN	C8'-N1-C2	2.98	121.25	117.86
1	B	2001	GPN	N2-C2-N3	3.13	123.53	117.75
1	C	3004	APN	C2'-C3'-N4'	3.35	119.53	113.44
1	C	3003	CPN	C5-C6-N1	3.36	124.21	121.35
1	B	2002	GPN	C8'-C7'-N4'	3.88	122.16	117.05
1	A	1006	GPN	C8'-N9-C8	4.06	130.48	125.67
1	A	1006	GPN	N2-C2-N3	4.20	125.51	117.75
1	B	2002	GPN	C6-N1-C2	4.40	122.39	116.06
1	B	2006	GPN	C6-N1-C2	4.62	122.71	116.06
1	B	2001	GPN	C6-N1-C2	4.81	122.98	116.06
1	C	3001	GPN	C6-N1-C2	5.05	123.33	116.06
1	C	3002	GPN	C6-N1-C2	5.22	123.58	116.06
1	D	4001	GPN	C6-N1-C2	5.79	124.38	116.06
1	C	3006	GPN	C6-N1-C2	5.80	124.40	116.06
1	D	4002	GPN	C6-N1-C2	5.96	124.63	116.06
1	A	1001	GPN	C6-N1-C2	6.22	125.01	116.06
1	A	1002	GPN	C6-N1-C2	6.26	125.07	116.06
1	D	4006	GPN	C6-N1-C2	6.98	126.10	116.06
1	D	4005	TPN	C2'-C3'-N4'	9.34	130.41	113.44
1	C	3005	TPN	C4-N3-C2	10.42	124.27	115.16
1	D	4005	TPN	C4-N3-C2	11.03	124.80	115.16
1	B	2005	TPN	C4-N3-C2	12.00	125.66	115.16
1	A	1005	TPN	C4-N3-C2	12.31	125.92	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	4004	APN	1	0

## 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	$\# Z  > 2$
2	EDO	A	5003	-	3,3,3	0.74	0	2,2,2	0.54	0
2	EDO	A	5005	-	3,3,3	0.74	0	2,2,2	0.60	0
2	EDO	B	5004	-	3,3,3	0.53	0	2,2,2	0.43	0
2	EDO	D	5001	-	3,3,3	0.61	0	2,2,2	0.20	0
2	EDO	D	5002	-	3,3,3	0.54	0	2,2,2	0.28	0

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	EDO	A	5003	-	-	0/1/1/1	0/0/0/0
2	EDO	A	5005	-	-	0/1/1/1	0/0/0/0
2	EDO	B	5004	-	-	0/1/1/1	0/0/0/0
2	EDO	D	5001	-	-	0/1/1/1	0/0/0/0
2	EDO	D	5002	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	1/9 (11%)	0.44	0 100 100	37, 37, 37, 37	0
1	B	0/9	-	-	-	-
1	C	1/9 (11%)	0.02	0 100 100	17, 17, 17, 17	0
1	D	0/9	-	-	-	-
All	All	2/36 (5%)	0.23	0 100 100	17, 17, 17, 37	0

There are no RSRZ outliers to report.

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPN	A	1005	19/20	0.96	0.07	-	12,15,20,20	0
1	CPN	B	2008	18/19	0.97	0.06	-	8,10,18,18	0
1	GPN	A	1001	21/22	0.97	0.06	-	9,12,16,16	0
1	APN	D	4004	20/21	0.97	0.06	-	9,12,19,25	0
1	GPN	A	1002	21/22	0.97	0.06	-	8,10,12,12	0
1	GPN	D	4001	19/22	0.97	0.06	-	11,13,15,18	0
1	TPN	B	2005	19/20	0.98	0.05	-	11,13,19,19	0
1	TPN	C	3005	19/20	0.98	0.06	-	11,14,19,19	0
1	CPN	D	4007	18/19	0.96	0.08	-	13,15,22,23	0
1	GPN	B	2002	21/22	0.97	0.05	-	13,16,17,18	0
1	APN	C	3004	20/21	0.97	0.06	-	11,14,19,22	0
1	GPN	B	2006	21/22	0.97	0.06	-	7,8,10,11	0
1	CPN	D	4008	16/19	0.97	0.06	-	14,16,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	GPN	C	3001	21/22	0.96	0.07	-	14,17,21,23	0
1	CPN	A	1003	18/19	0.97	0.06	-	8,10,15,18	0
1	APN	A	1004	20/21	0.97	0.06	-	10,11,18,31	0
1	CPN	B	2007	18/19	0.98	0.06	-	7,8,10,11	0
1	CPN	B	2003	18/19	0.98	0.06	-	11,14,17,21	0
1	GPN	A	1006	21/22	0.97	0.07	-	12,14,18,23	0
1	APN	B	2004	20/21	0.97	0.06	-	13,14,22,23	0
1	GPN	C	3006	21/22	0.98	0.05	-	7,9,11,11	0
1	GPN	D	4006	21/22	0.96	0.08	-	11,14,20,26	0
1	CPN	A	1007	18/19	0.97	0.07	-	13,15,22,32	0
1	CPN	C	3003	18/19	0.97	0.06	-	12,14,18,21	0
1	CPN	A	1008	18/19	0.95	0.07	-	14,17,25,48	0
1	CPN	C	3007	18/19	0.98	0.06	-	6,8,11,11	0
1	GPN	B	2001	21/22	0.96	0.07	-	15,18,19,20	0
1	GPN	C	3002	21/22	0.97	0.06	-	13,15,17,18	0
1	TPN	D	4005	19/20	0.96	0.07	-	14,16,20,23	0
1	CPN	D	4003	18/19	0.98	0.06	-	9,10,12,13	0
1	GPN	D	4002	21/22	0.98	0.06	-	8,10,11,12	0
1	CPN	C	3008	18/19	0.96	0.07	-	8,10,13,21	0

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	A	5005	4/4	0.96	0.08	-	16,22,27,27	0
2	EDO	A	5003	4/4	0.99	0.06	-	10,12,12,12	0
2	EDO	D	5001	4/4	0.98	0.06	-	11,13,14,14	0
2	EDO	D	5002	4/4	0.98	0.06	-	13,14,15,17	0
2	EDO	B	5004	4/4	0.95	0.07	-	17,19,19,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.