



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 11:48 AM UTC

PDB ID : 1RRU / pdb_00001rru
Title : The influence of a chiral amino acid on the helical handedness of PNA in solution and in crystals
Authors : Rasmussen, H.; Liljefors, T.; Petersson, B.; Nielsen, P.E.; Kastrup, J.S.
Deposited on : 2003-12-09
Resolution : 2.35 Å(reported)

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

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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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

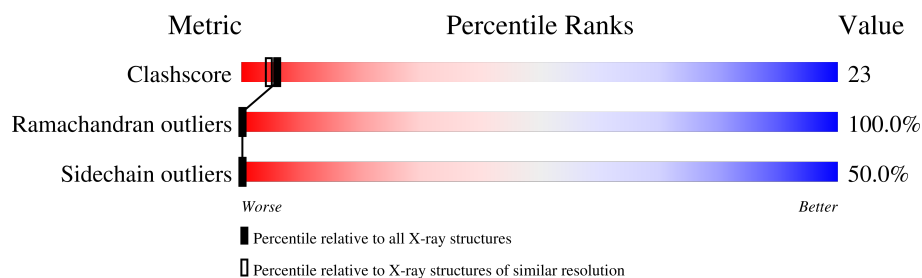
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

ENTRY-COMPOSITION INFOmissingINFO

2 Residue-property plots

There is no protein, DNA or RNA chain in this entry to show sequence plots.

3 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	36.75 Å 44.07 Å 31.22 Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	6.00 – 2.35	Depositor
% Data completeness (in resolution range)	74.0 (6.00-2.35)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.219 , 0.292	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	294	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, APN, CPN, TPN, GPN

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	0.85	0/8	1.97	0/8
1	B	1.81	0/8	2.65	0/8
All	All	1.42	0/16	2.33	0/16

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	133	0	49	5	0
1	B	133	0	49	0	0
2	A	15	0	0	9	0
2	B	13	0	0	0	0
All	All	294	0	98	9	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 23.

All (9) 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:5:CPN:N	2:A:29:HOH:O	2.29	0.65
1:A:4[B]:APN:C3'	2:A:29:HOH:O	2.47	0.61
1:A:4[A]:APN:C3'	2:A:29:HOH:O	2.49	0.59
1:A:5:CPN:C7'	2:A:30:HOH:O	2.57	0.53
1:A:6:GPN:H8'1	2:A:30:HOH:O	2.17	0.42

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

4.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

16 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	2	1	22,22,23	1.29	4 (18%)	29,30,32	1.14	3 (10%)
1	TPN	B	11[A]	1	19,19,20	1.79	4 (21%)	24,25,27	3.25	14 (58%)
1	GPN	B	10	1	22,22,23	1.13	0	29,30,32	2.03	9 (31%)
1	APN	A	4[A]	1	21,21,22	1.65	3 (14%)	27,28,30	1.77	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CPN	A	5	1	18,18,19	0.93	1 (5%)	21,23,25	1.80	6 (28%)
1	CPN	B	13	1	18,18,19	1.36	2 (11%)	21,23,25	2.10	6 (28%)
1	APN	B	12[B]	1	21,21,22	1.56	4 (19%)	27,28,30	2.47	9 (33%)
1	GPN	A	6	1	22,22,23	1.00	1 (4%)	29,30,32	0.93	0
1	CPN	A	1	1	18,18,19	1.30	3 (16%)	21,23,25	2.00	4 (19%)
1	TPN	A	3[B]	1	19,19,20	1.24	3 (15%)	24,25,27	1.98	5 (20%)
1	TPN	B	11[B]	1	19,19,20	1.73	3 (15%)	24,25,27	3.23	13 (54%)
1	CPN	B	9	1	18,18,19	1.63	3 (16%)	21,23,25	2.21	7 (33%)
1	APN	B	12[A]	1	21,21,22	1.56	4 (19%)	27,28,30	2.48	9 (33%)
1	TPN	A	3[A]	1	19,19,20	1.24	3 (15%)	24,25,27	1.99	5 (20%)
1	GPN	B	14	1	22,22,23	1.43	3 (13%)	29,30,32	1.82	5 (17%)
1	APN	A	4[B]	1	21,21,22	1.65	3 (14%)	27,28,30	1.74	7 (25%)

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	2	1	-	0/13/14/15	0/2/2/2
1	TPN	B	11[A]	1	-	0/13/14/15	0/1/1/1
1	GPN	B	10	1	-	0/13/14/15	0/2/2/2
1	APN	A	4[A]	1	-	0/13/14/15	0/2/2/2
1	CPN	A	5	1	-	0/13/14/15	0/1/1/1
1	CPN	B	13	1	-	2/13/14/15	0/1/1/1
1	APN	B	12[B]	1	-	1/13/14/15	0/2/2/2
1	GPN	A	6	1	-	1/13/14/15	0/2/2/2
1	CPN	A	1	1	-	1/13/14/15	0/1/1/1
1	TPN	A	3[B]	1	-	3/13/14/15	0/1/1/1
1	TPN	B	11[B]	1	-	1/13/14/15	0/1/1/1
1	CPN	B	9	1	-	0/13/14/15	0/1/1/1
1	APN	B	12[A]	1	-	0/13/14/15	0/2/2/2
1	TPN	A	3[A]	1	-	1/13/14/15	0/1/1/1
1	GPN	B	14	1	-	1/13/14/15	0/2/2/2
1	APN	A	4[B]	1	-	1/13/14/15	0/2/2/2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4[A]	APN	C4-N9	-4.93	1.31	1.37
1	A	4[B]	APN	C4-N9	-4.93	1.31	1.37
1	B	11[A]	TPN	C2-N1	4.74	1.44	1.37
1	B	11[B]	TPN	C2-N1	4.74	1.44	1.37
1	B	9	CPN	C6-N1	-4.03	1.31	1.37
1	A	4[A]	APN	C8'-N9	-3.94	1.41	1.46
1	A	4[B]	APN	C8'-N9	-3.94	1.41	1.46
1	B	13	CPN	C2-N1	-3.62	1.35	1.40
1	B	11[A]	TPN	C8'-C7'	-3.46	1.48	1.53
1	B	11[B]	TPN	C8'-C7'	-3.46	1.48	1.53
1	B	12[A]	APN	C4-N3	-3.35	1.28	1.34
1	B	12[B]	APN	C4-N3	-3.35	1.28	1.34
1	A	3[A]	TPN	C8'-C7'	-3.28	1.48	1.53
1	A	3[B]	TPN	C8'-C7'	-3.28	1.48	1.53
1	B	14	GPN	C8'-C7'	3.18	1.57	1.53
1	B	9	CPN	C8'-N1	-3.14	1.42	1.46
1	A	6	GPN	C3'-C2'	3.10	1.64	1.50
1	A	2	GPN	C7'-N4'	-2.91	1.29	1.35
1	B	12[A]	APN	C2-N1	-2.81	1.28	1.33
1	B	12[B]	APN	C2-N1	-2.81	1.28	1.33
1	B	14	GPN	C3'-C2'	2.79	1.62	1.50
1	B	13	CPN	C8'-C7'	2.78	1.57	1.53
1	B	12[A]	APN	C5-C4	-2.76	1.34	1.39
1	B	12[B]	APN	C5-C4	-2.76	1.34	1.39
1	B	14	GPN	C4-N9	-2.59	1.33	1.37
1	A	1	CPN	C8'-N1	2.52	1.49	1.46
1	A	3[B]	TPN	C5'-C	2.43	1.57	1.49
1	A	2	GPN	C5-C6	-2.42	1.35	1.44
1	A	1	CPN	C8'-C7'	-2.34	1.49	1.53
1	A	3[A]	TPN	C5'-C	2.30	1.57	1.49
1	A	1	CPN	C7'-N4'	-2.28	1.30	1.35
1	B	11[A]	TPN	C5'-C	2.24	1.57	1.49
1	A	2	GPN	C5'-C	2.18	1.57	1.49
1	A	4[A]	APN	C5-C4	-2.15	1.35	1.39
1	A	4[B]	APN	C5-C4	-2.15	1.35	1.39
1	B	11[A]	TPN	C5M-C5	-2.10	1.45	1.50
1	B	11[B]	TPN	C5M-C5	-2.10	1.45	1.50
1	B	12[A]	APN	C8-N7	2.10	1.35	1.31
1	B	12[B]	APN	C8-N7	2.10	1.35	1.31
1	A	3[A]	TPN	C2-N1	2.06	1.40	1.37
1	A	3[B]	TPN	C2-N1	2.06	1.40	1.37
1	B	9	CPN	C3'-C2'	2.05	1.59	1.50
1	A	2	GPN	C4-N9	2.00	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	CPN	C2-N1	-2.00	1.37	1.40

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11[A]	TPN	C6-C5-C4	7.14	123.91	118.02
1	B	11[B]	TPN	C6-C5-C4	7.14	123.91	118.02
1	B	12[A]	APN	C8'-C7'-N4'	7.10	125.66	117.04
1	B	12[B]	APN	C8'-C7'-N4'	7.10	125.66	117.04
1	B	11[A]	TPN	C7'-C8'-N1	6.26	119.19	110.73
1	B	11[B]	TPN	C7'-C8'-N1	6.26	119.19	110.73
1	A	3[A]	TPN	C6-C5-C4	5.87	122.86	118.02
1	A	3[B]	TPN	C6-C5-C4	5.87	122.86	118.02
1	B	13	CPN	O2-C2-N1	5.86	124.70	119.17
1	B	12[A]	APN	N9-C8-N7	-5.84	108.76	114.16
1	B	12[B]	APN	N9-C8-N7	-5.84	108.76	114.16
1	B	11[A]	TPN	C5M-C5-C6	-5.74	115.08	122.85
1	B	11[B]	TPN	C5M-C5-C6	-5.74	115.08	122.85
1	A	1	CPN	C8'-C7'-N4'	5.68	123.93	117.04
1	B	9	CPN	C7'-C8'-N1	5.57	118.26	110.73
1	B	14	GPN	C7'-C8'-N9	-5.51	103.28	110.73
1	B	10	GPN	C8'-C7'-N4'	5.13	123.27	117.04
1	B	11[A]	TPN	O2-C2-N1	5.00	127.11	122.87
1	B	11[B]	TPN	O2-C2-N1	5.00	127.11	122.87
1	B	9	CPN	O2-C2-N1	4.65	123.56	119.17
1	B	11[A]	TPN	N3-C2-N1	4.49	118.72	114.86
1	B	11[B]	TPN	N3-C2-N1	4.49	118.72	114.86
1	B	10	GPN	C8'-N9-C8	4.47	133.29	126.49
1	A	5	CPN	C8'-C7'-N4'	4.29	122.25	117.04
1	B	12[A]	APN	C8'-N9-C8	4.24	131.47	127.27
1	B	12[B]	APN	C8'-N9-C8	4.24	131.47	127.27
1	B	14	GPN	C8'-C7'-N4'	4.14	122.07	117.04
1	B	13	CPN	O2-C2-N3	-4.01	116.01	122.33
1	B	11[A]	TPN	O2-C2-N3	-3.97	114.17	121.49
1	B	11[B]	TPN	O2-C2-N3	-3.97	114.17	121.49
1	A	4[A]	APN	C8'-N9-C8	3.93	131.17	127.27
1	A	4[B]	APN	C8'-N9-C8	3.93	131.17	127.27
1	A	4[A]	APN	C2'-C3'-N4'	-3.53	104.99	112.91
1	A	4[B]	APN	C2'-C3'-N4'	-3.50	105.05	112.91
1	B	13	CPN	C2'-C3'-N4'	-3.43	105.22	112.91
1	B	9	CPN	C5-C4-N4	-3.42	114.64	120.63
1	A	1	CPN	C8'-N1-C6	3.40	124.65	119.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3[A]	TPN	C5M-C5-C6	-3.38	118.28	122.85
1	A	3[B]	TPN	C5M-C5-C6	-3.38	118.28	122.85
1	B	10	GPN	C5'-N4'-C3'	-3.34	112.31	117.06
1	B	12[A]	APN	C8'-N9-C4	-3.33	122.00	126.04
1	B	12[B]	APN	C8'-N9-C4	-3.33	122.00	126.04
1	A	4[A]	APN	C8'-C7'-N4'	3.32	121.06	117.04
1	A	4[B]	APN	C8'-C7'-N4'	3.32	121.06	117.04
1	B	11[A]	TPN	C5-C6-N1	-3.29	119.90	123.54
1	B	11[B]	TPN	C5-C6-N1	-3.29	119.90	123.54
1	A	5	CPN	C8'-N1-C6	3.23	124.41	119.72
1	B	11[A]	TPN	O4-C4-C5	3.18	128.55	124.92
1	B	11[B]	TPN	O4-C4-C5	3.18	128.55	124.92
1	B	10	GPN	C2'-C3'-N4'	-3.15	105.82	112.91
1	B	9	CPN	N4-C4-N3	3.15	123.53	117.91
1	A	3[A]	TPN	N3-C2-N1	3.05	117.48	114.86
1	A	3[B]	TPN	N3-C2-N1	3.05	117.48	114.86
1	A	3[A]	TPN	C5-C6-N1	-3.03	120.19	123.54
1	A	3[B]	TPN	C5-C6-N1	-3.03	120.19	123.54
1	A	4[A]	APN	C8'-N9-C4	-2.98	122.42	126.04
1	A	4[B]	APN	C8'-N9-C4	-2.98	122.42	126.04
1	A	5	CPN	O7'-C7'-N4'	-2.98	116.82	122.12
1	A	3[A]	TPN	C8'-N1-C6	2.97	123.99	120.20
1	A	3[B]	TPN	C8'-N1-C6	2.97	123.99	120.20
1	B	12[A]	APN	O7'-C7'-N4'	-2.96	116.86	122.12
1	B	12[B]	APN	O7'-C7'-N4'	-2.96	116.86	122.12
1	A	4[A]	APN	N9-C8-N7	-2.92	111.46	114.16
1	A	4[B]	APN	N9-C8-N7	-2.92	111.46	114.16
1	B	10	GPN	O7'-C7'-N4'	-2.90	116.96	122.12
1	A	1	CPN	O7'-C7'-N4'	-2.90	116.96	122.12
1	A	2	GPN	O7'-C7'-N4'	-2.85	117.06	122.12
1	A	1	CPN	C5-C4-N4	-2.79	115.74	120.63
1	B	13	CPN	O7'-C7'-C8'	2.75	124.64	120.56
1	B	11[A]	TPN	C4-N3-C2	-2.72	123.78	127.34
1	B	11[B]	TPN	C4-N3-C2	-2.72	123.78	127.34
1	B	13	CPN	O7'-C7'-N4'	-2.71	117.30	122.12
1	B	9	CPN	C8'-C7'-N4'	-2.70	113.76	117.04
1	B	11[A]	TPN	C5'-N4'-C3'	-2.69	113.23	117.06
1	B	12[A]	APN	C2-N1-C6	-2.68	114.33	118.73
1	B	12[B]	APN	C2-N1-C6	-2.68	114.33	118.73
1	B	11[A]	TPN	C6-N1-C2	-2.67	118.65	121.29
1	B	11[B]	TPN	C6-N1-C2	-2.67	118.65	121.29
1	B	11[A]	TPN	C8'-N1-C6	2.62	123.55	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11[B]	TPN	C8'-N1-C6	2.62	123.55	120.20
1	B	10	GPN	C8'-N9-C4	-2.61	123.44	127.02
1	B	12[A]	APN	C5-C4-N9	2.57	108.61	105.98
1	B	12[B]	APN	C5-C4-N9	2.57	108.61	105.98
1	B	14	GPN	C5'-N4'-C3'	2.51	120.63	117.06
1	B	12[B]	APN	C2'-C3'-N4'	-2.49	107.33	112.91
1	B	13	CPN	C7'-C8'-N1	2.47	114.07	110.73
1	A	5	CPN	O2-C2-N1	2.46	121.49	119.17
1	B	10	GPN	C8-N9-C4	-2.43	103.26	105.89
1	B	11[A]	TPN	C8'-C7'-N4'	2.38	119.93	117.04
1	B	11[B]	TPN	C8'-C7'-N4'	2.38	119.93	117.04
1	A	5	CPN	C2'-C3'-N4'	-2.36	107.62	112.91
1	B	10	GPN	N9-C4-N3	-2.32	122.06	125.46
1	B	14	GPN	N2-C2-N1	2.29	121.59	116.76
1	A	4[A]	APN	C5'-N4'-C3'	-2.28	113.82	117.06
1	A	2	GPN	O7'-C7'-C8'	2.25	123.90	120.56
1	B	10	GPN	C2-N3-C4	-2.24	108.43	112.30
1	A	4[A]	APN	C5-C4-N9	2.24	108.28	105.98
1	A	4[B]	APN	C5-C4-N9	2.24	108.28	105.98
1	B	12[A]	APN	C2'-C3'-N4'	-2.23	107.91	112.91
1	A	4[A]	APN	C7'-C8'-N9	-2.22	107.91	110.81
1	A	4[B]	APN	C7'-C8'-N9	-2.22	107.91	110.81
1	B	14	GPN	C2-N3-C4	2.22	116.12	112.30
1	B	9	CPN	O7'-C7'-C8'	2.17	123.78	120.56
1	B	9	CPN	C6-N1-C2	2.11	122.21	120.06
1	B	11[A]	TPN	C5M-C5-C4	2.09	121.02	118.78
1	B	11[B]	TPN	C5M-C5-C4	2.09	121.02	118.78
1	B	12[A]	APN	O7'-C7'-C8'	-2.09	117.48	120.56
1	B	12[B]	APN	O7'-C7'-C8'	-2.09	117.48	120.56
1	A	2	GPN	C8-N9-C4	-2.07	103.66	105.89
1	A	5	CPN	C7'-C8'-N1	2.05	113.50	110.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	CPN	N-C2'-C3'-N4'
1	A	3[B]	TPN	C-C5'-N4'-C7'
1	A	4[B]	APN	N-C2'-C3'-N4'
1	B	12[B]	APN	N-C2'-C3'-N4'
1	B	11[B]	TPN	C-C5'-N4'-C7'
1	A	6	GPN	C7'-C8'-N9-C4

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Mol	Chain	Res	Type	Atoms
1	B	14	GPN	C7'-C8'-N9-C4
1	A	3[B]	TPN	C-C5'-N4'-C3'
1	B	13	CPN	C7'-C8'-N1-C6
1	A	3[A]	TPN	C7'-C8'-N1-C2
1	A	3[B]	TPN	C7'-C8'-N1-C2
1	B	13	CPN	C7'-C8'-N1-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	4[A]	APN	1	0
1	A	5	CPN	2	0
1	A	6	GPN	1	0
1	A	4[B]	APN	1	0

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

Of 20 such residues modelled in this entry, 2 are modelled with single atom - leaving 18 for Mogul analysis.

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	2	1	22,22,23	1.29	4 (18%)	29,30,32	1.14	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPN	B	11[A]	1	19,19,20	1.79	4 (21%)	24,25,27	3.25	14 (58%)
1	GPN	B	10	1	22,22,23	1.13	0	29,30,32	2.03	9 (31%)
1	APN	A	4[A]	1	21,21,22	1.65	3 (14%)	27,28,30	1.77	8 (29%)
1	CPN	A	5	1	18,18,19	0.93	1 (5%)	21,23,25	1.80	6 (28%)
1	CPN	B	13	1	18,18,19	1.36	2 (11%)	21,23,25	2.10	6 (28%)
1	APN	B	12[B]	1	21,21,22	1.56	4 (19%)	27,28,30	2.47	9 (33%)
1	GPN	A	6	1	22,22,23	1.00	1 (4%)	29,30,32	0.93	0
1	CPN	A	1	1	18,18,19	1.30	3 (16%)	21,23,25	2.00	4 (19%)
1	TPN	A	3[B]	1	19,19,20	1.24	3 (15%)	24,25,27	1.98	5 (20%)
1	TPN	B	11[B]	1	19,19,20	1.73	3 (15%)	24,25,27	3.23	13 (54%)
1	CPN	B	9	1	18,18,19	1.63	3 (16%)	21,23,25	2.21	7 (33%)
1	APN	B	12[A]	1	21,21,22	1.56	4 (19%)	27,28,30	2.48	9 (33%)
1	TPN	A	3[A]	1	19,19,20	1.24	3 (15%)	24,25,27	1.99	5 (20%)
1	GPN	B	14	1	22,22,23	1.43	3 (13%)	29,30,32	1.82	5 (17%)
1	APN	A	4[B]	1	21,21,22	1.65	3 (14%)	27,28,30	1.74	7 (25%)

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	2	1	-	0/13/14/15	0/2/2/2
1	TPN	B	11[A]	1	-	0/13/14/15	0/1/1/1
1	GPN	B	10	1	-	0/13/14/15	0/2/2/2
1	APN	A	4[A]	1	-	0/13/14/15	0/2/2/2
1	CPN	A	5	1	-	0/13/14/15	0/1/1/1
1	CPN	B	13	1	-	2/13/14/15	0/1/1/1
1	APN	B	12[B]	1	-	1/13/14/15	0/2/2/2
1	GPN	A	6	1	-	1/13/14/15	0/2/2/2
1	CPN	A	1	1	-	1/13/14/15	0/1/1/1
1	TPN	A	3[B]	1	-	3/13/14/15	0/1/1/1
1	TPN	B	11[B]	1	-	1/13/14/15	0/1/1/1
1	CPN	B	9	1	-	0/13/14/15	0/1/1/1
1	APN	B	12[A]	1	-	0/13/14/15	0/2/2/2
1	TPN	A	3[A]	1	-	1/13/14/15	0/1/1/1
1	GPN	B	14	1	-	1/13/14/15	0/2/2/2
1	APN	A	4[B]	1	-	1/13/14/15	0/2/2/2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4[A]	APN	C4-N9	-4.93	1.31	1.37
1	A	4[B]	APN	C4-N9	-4.93	1.31	1.37
1	B	11[A]	TPN	C2-N1	4.74	1.44	1.37
1	B	11[B]	TPN	C2-N1	4.74	1.44	1.37
1	B	9	CPN	C6-N1	-4.03	1.31	1.37
1	A	4[A]	APN	C8'-N9	-3.94	1.41	1.46
1	A	4[B]	APN	C8'-N9	-3.94	1.41	1.46
1	B	13	CPN	C2-N1	-3.62	1.35	1.40
1	B	11[A]	TPN	C8'-C7'	-3.46	1.48	1.53
1	B	11[B]	TPN	C8'-C7'	-3.46	1.48	1.53
1	B	12[A]	APN	C4-N3	-3.35	1.28	1.34
1	B	12[B]	APN	C4-N3	-3.35	1.28	1.34
1	A	3[A]	TPN	C8'-C7'	-3.28	1.48	1.53
1	A	3[B]	TPN	C8'-C7'	-3.28	1.48	1.53
1	B	14	GPN	C8'-C7'	3.18	1.57	1.53
1	B	9	CPN	C8'-N1	-3.14	1.42	1.46
1	A	6	GPN	C3'-C2'	3.10	1.64	1.50
1	A	2	GPN	C7'-N4'	-2.91	1.29	1.35
1	B	12[A]	APN	C2-N1	-2.81	1.28	1.33
1	B	12[B]	APN	C2-N1	-2.81	1.28	1.33
1	B	14	GPN	C3'-C2'	2.79	1.62	1.50
1	B	13	CPN	C8'-C7'	2.78	1.57	1.53
1	B	12[A]	APN	C5-C4	-2.76	1.34	1.39
1	B	12[B]	APN	C5-C4	-2.76	1.34	1.39
1	B	14	GPN	C4-N9	-2.59	1.33	1.37
1	A	1	CPN	C8'-N1	2.52	1.49	1.46
1	A	3[B]	TPN	C5'-C	2.43	1.57	1.49
1	A	2	GPN	C5-C6	-2.42	1.35	1.44
1	A	1	CPN	C8'-C7'	-2.34	1.49	1.53
1	A	3[A]	TPN	C5'-C	2.30	1.57	1.49
1	A	1	CPN	C7'-N4'	-2.28	1.30	1.35
1	B	11[A]	TPN	C5'-C	2.24	1.57	1.49
1	A	2	GPN	C5'-C	2.18	1.57	1.49
1	A	4[A]	APN	C5-C4	-2.15	1.35	1.39
1	A	4[B]	APN	C5-C4	-2.15	1.35	1.39
1	B	11[A]	TPN	C5M-C5	-2.10	1.45	1.50
1	B	11[B]	TPN	C5M-C5	-2.10	1.45	1.50
1	B	12[A]	APN	C8-N7	2.10	1.35	1.31
1	B	12[B]	APN	C8-N7	2.10	1.35	1.31
1	A	3[A]	TPN	C2-N1	2.06	1.40	1.37
1	A	3[B]	TPN	C2-N1	2.06	1.40	1.37
1	B	9	CPN	C3'-C2'	2.05	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	GPN	C4-N9	2.00	1.40	1.37
1	A	5	CPN	C2-N1	-2.00	1.37	1.40

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11[A]	TPN	C6-C5-C4	7.14	123.91	118.02
1	B	11[B]	TPN	C6-C5-C4	7.14	123.91	118.02
1	B	12[A]	APN	C8'-C7'-N4'	7.10	125.66	117.04
1	B	12[B]	APN	C8'-C7'-N4'	7.10	125.66	117.04
1	B	11[A]	TPN	C7'-C8'-N1	6.26	119.19	110.73
1	B	11[B]	TPN	C7'-C8'-N1	6.26	119.19	110.73
1	A	3[A]	TPN	C6-C5-C4	5.87	122.86	118.02
1	A	3[B]	TPN	C6-C5-C4	5.87	122.86	118.02
1	B	13	CPN	O2-C2-N1	5.86	124.70	119.17
1	B	12[A]	APN	N9-C8-N7	-5.84	108.76	114.16
1	B	12[B]	APN	N9-C8-N7	-5.84	108.76	114.16
1	B	11[A]	TPN	C5M-C5-C6	-5.74	115.08	122.85
1	B	11[B]	TPN	C5M-C5-C6	-5.74	115.08	122.85
1	A	1	CPN	C8'-C7'-N4'	5.68	123.93	117.04
1	B	9	CPN	C7'-C8'-N1	5.57	118.26	110.73
1	B	14	GPN	C7'-C8'-N9	-5.51	103.28	110.73
1	B	10	GPN	C8'-C7'-N4'	5.13	123.27	117.04
1	B	11[A]	TPN	O2-C2-N1	5.00	127.11	122.87
1	B	11[B]	TPN	O2-C2-N1	5.00	127.11	122.87
1	B	9	CPN	O2-C2-N1	4.65	123.56	119.17
1	B	11[A]	TPN	N3-C2-N1	4.49	118.72	114.86
1	B	11[B]	TPN	N3-C2-N1	4.49	118.72	114.86
1	B	10	GPN	C8'-N9-C8	4.47	133.29	126.49
1	A	5	CPN	C8'-C7'-N4'	4.29	122.25	117.04
1	B	12[A]	APN	C8'-N9-C8	4.24	131.47	127.27
1	B	12[B]	APN	C8'-N9-C8	4.24	131.47	127.27
1	B	14	GPN	C8'-C7'-N4'	4.14	122.07	117.04
1	B	13	CPN	O2-C2-N3	-4.01	116.01	122.33
1	B	11[A]	TPN	O2-C2-N3	-3.97	114.17	121.49
1	B	11[B]	TPN	O2-C2-N3	-3.97	114.17	121.49
1	A	4[A]	APN	C8'-N9-C8	3.93	131.17	127.27
1	A	4[B]	APN	C8'-N9-C8	3.93	131.17	127.27
1	A	4[A]	APN	C2'-C3'-N4'	-3.53	104.99	112.91
1	A	4[B]	APN	C2'-C3'-N4'	-3.50	105.05	112.91
1	B	13	CPN	C2'-C3'-N4'	-3.43	105.22	112.91
1	B	9	CPN	C5-C4-N4	-3.42	114.64	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	CPN	C8'-N1-C6	3.40	124.65	119.72
1	A	3[A]	TPN	C5M-C5-C6	-3.38	118.28	122.85
1	A	3[B]	TPN	C5M-C5-C6	-3.38	118.28	122.85
1	B	10	GPN	C5'-N4'-C3'	-3.34	112.31	117.06
1	B	12[A]	APN	C8'-N9-C4	-3.33	122.00	126.04
1	B	12[B]	APN	C8'-N9-C4	-3.33	122.00	126.04
1	A	4[A]	APN	C8'-C7'-N4'	3.32	121.06	117.04
1	A	4[B]	APN	C8'-C7'-N4'	3.32	121.06	117.04
1	B	11[A]	TPN	C5-C6-N1	-3.29	119.90	123.54
1	B	11[B]	TPN	C5-C6-N1	-3.29	119.90	123.54
1	A	5	CPN	C8'-N1-C6	3.23	124.41	119.72
1	B	11[A]	TPN	O4-C4-C5	3.18	128.55	124.92
1	B	11[B]	TPN	O4-C4-C5	3.18	128.55	124.92
1	B	10	GPN	C2'-C3'-N4'	-3.15	105.82	112.91
1	B	9	CPN	N4-C4-N3	3.15	123.53	117.91
1	A	3[A]	TPN	N3-C2-N1	3.05	117.48	114.86
1	A	3[B]	TPN	N3-C2-N1	3.05	117.48	114.86
1	A	3[A]	TPN	C5-C6-N1	-3.03	120.19	123.54
1	A	3[B]	TPN	C5-C6-N1	-3.03	120.19	123.54
1	A	4[A]	APN	C8'-N9-C4	-2.98	122.42	126.04
1	A	4[B]	APN	C8'-N9-C4	-2.98	122.42	126.04
1	A	5	CPN	O7'-C7'-N4'	-2.98	116.82	122.12
1	A	3[A]	TPN	C8'-N1-C6	2.97	123.99	120.20
1	A	3[B]	TPN	C8'-N1-C6	2.97	123.99	120.20
1	B	12[A]	APN	O7'-C7'-N4'	-2.96	116.86	122.12
1	B	12[B]	APN	O7'-C7'-N4'	-2.96	116.86	122.12
1	A	4[A]	APN	N9-C8-N7	-2.92	111.46	114.16
1	A	4[B]	APN	N9-C8-N7	-2.92	111.46	114.16
1	B	10	GPN	O7'-C7'-N4'	-2.90	116.96	122.12
1	A	1	CPN	O7'-C7'-N4'	-2.90	116.96	122.12
1	A	2	GPN	O7'-C7'-N4'	-2.85	117.06	122.12
1	A	1	CPN	C5-C4-N4	-2.79	115.74	120.63
1	B	13	CPN	O7'-C7'-C8'	2.75	124.64	120.56
1	B	11[A]	TPN	C4-N3-C2	-2.72	123.78	127.34
1	B	11[B]	TPN	C4-N3-C2	-2.72	123.78	127.34
1	B	13	CPN	O7'-C7'-N4'	-2.71	117.30	122.12
1	B	9	CPN	C8'-C7'-N4'	-2.70	113.76	117.04
1	B	11[A]	TPN	C5'-N4'-C3'	-2.69	113.23	117.06
1	B	12[A]	APN	C2-N1-C6	-2.68	114.33	118.73
1	B	12[B]	APN	C2-N1-C6	-2.68	114.33	118.73
1	B	11[A]	TPN	C6-N1-C2	-2.67	118.65	121.29
1	B	11[B]	TPN	C6-N1-C2	-2.67	118.65	121.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11[A]	TPN	C8'-N1-C6	2.62	123.55	120.20
1	B	11[B]	TPN	C8'-N1-C6	2.62	123.55	120.20
1	B	10	GPN	C8'-N9-C4	-2.61	123.44	127.02
1	B	12[A]	APN	C5-C4-N9	2.57	108.61	105.98
1	B	12[B]	APN	C5-C4-N9	2.57	108.61	105.98
1	B	14	GPN	C5'-N4'-C3'	2.51	120.63	117.06
1	B	12[B]	APN	C2'-C3'-N4'	-2.49	107.33	112.91
1	B	13	CPN	C7'-C8'-N1	2.47	114.07	110.73
1	A	5	CPN	O2-C2-N1	2.46	121.49	119.17
1	B	10	GPN	C8-N9-C4	-2.43	103.26	105.89
1	B	11[A]	TPN	C8'-C7'-N4'	2.38	119.93	117.04
1	B	11[B]	TPN	C8'-C7'-N4'	2.38	119.93	117.04
1	A	5	CPN	C2'-C3'-N4'	-2.36	107.62	112.91
1	B	10	GPN	N9-C4-N3	-2.32	122.06	125.46
1	B	14	GPN	N2-C2-N1	2.29	121.59	116.76
1	A	4[A]	APN	C5'-N4'-C3'	-2.28	113.82	117.06
1	A	2	GPN	O7'-C7'-C8'	2.25	123.90	120.56
1	B	10	GPN	C2-N3-C4	-2.24	108.43	112.30
1	A	4[A]	APN	C5-C4-N9	2.24	108.28	105.98
1	A	4[B]	APN	C5-C4-N9	2.24	108.28	105.98
1	B	12[A]	APN	C2'-C3'-N4'	-2.23	107.91	112.91
1	A	4[A]	APN	C7'-C8'-N9	-2.22	107.91	110.81
1	A	4[B]	APN	C7'-C8'-N9	-2.22	107.91	110.81
1	B	14	GPN	C2-N3-C4	2.22	116.12	112.30
1	B	9	CPN	O7'-C7'-C8'	2.17	123.78	120.56
1	B	9	CPN	C6-N1-C2	2.11	122.21	120.06
1	B	11[A]	TPN	C5M-C5-C4	2.09	121.02	118.78
1	B	11[B]	TPN	C5M-C5-C4	2.09	121.02	118.78
1	B	12[A]	APN	O7'-C7'-C8'	-2.09	117.48	120.56
1	B	12[B]	APN	O7'-C7'-C8'	-2.09	117.48	120.56
1	A	2	GPN	C8-N9-C4	-2.07	103.66	105.89
1	A	5	CPN	C7'-C8'-N1	2.05	113.50	110.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	CPN	N-C2'-C3'-N4'
1	A	3[B]	TPN	C-C5'-N4'-C7'
1	A	4[B]	APN	N-C2'-C3'-N4'
1	B	12[B]	APN	N-C2'-C3'-N4'
1	B	11[B]	TPN	C-C5'-N4'-C7'

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Mol	Chain	Res	Type	Atoms
1	A	6	GPN	C7'-C8'-N9-C4
1	B	14	GPN	C7'-C8'-N9-C4
1	A	3[B]	TPN	C-C5'-N4'-C3'
1	B	13	CPN	C7'-C8'-N1-C6
1	A	3[A]	TPN	C7'-C8'-N1-C2
1	A	3[B]	TPN	C7'-C8'-N1-C2
1	B	13	CPN	C7'-C8'-N1-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	4[A]	APN	1	0
1	A	5	CPN	2	0
1	A	6	GPN	1	0
1	A	4[B]	APN	1	0

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates

EDS was not executed - this section is therefore empty.

5.4 Ligands

EDS was not executed - this section is therefore empty.

5.5 Other polymers

EDS was not executed - this section is therefore empty.