



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:14 PM UTC

PDB ID : 1XJ9 / pdb_00001xj9
Title : Crystal structure of a partly self-complementary peptide nucleic acid (PNA) oligomer showing a duplex-triplex network
Authors : Petersson, B.; Nielsen, B.B.; Rasmussen, H.; Larsen, I.K.; Gajhede, M.; Nielsen, P.E.; Kastrup, J.S.
Deposited on : 2004-09-23
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

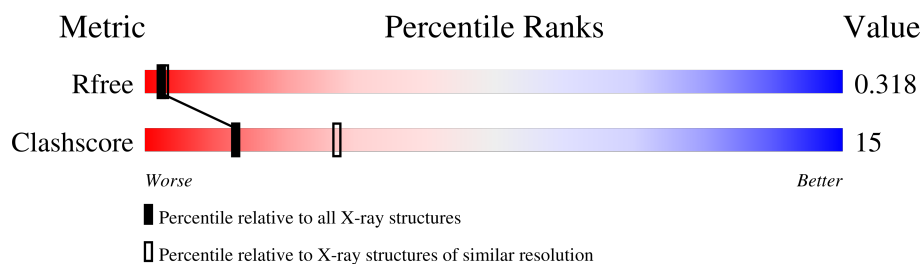
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	55.60Å 41.90Å 30.10Å 90.00° 117.70° 90.00°	Depositor
Resolution (Å)	27.00 – 2.60 27.00 – 2.63	Depositor EDS
% Data completeness (in resolution range)	78.2 (27.00-2.60) 98.2 (27.00-2.63)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 2.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.277 0.281 , 0.318	Depositor DCC
R_{free} test set	172 reflections (9.35%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.64$, $\langle L^2 \rangle = 0.51$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	413	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

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

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	190	0	51	4	0
1	B	190	0	50	4	0
2	A	19	0	0	1	0
2	B	14	0	0	0	0
All	All	413	0	101	8	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (8) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:11:HOH:O	1:B:203[A]:APN:H2	1.92	0.69
1:B:210:TPN:C	1:B:210:TPN:O7'	2.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107[B]:CPN:O	1:A:108[B]:APN:H3'2	2.09	0.53
1:B:207[B]:CPN:O	1:B:208[B]:APN:H3'1	2.09	0.52

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](#)

26 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	104[B]	1	22,22,23	0.67	0	29,30,32	1.06	2 (6%)
1	APN	B	208[B]	1	21,21,22	0.65	0	27,28,30	1.43	6 (22%)
1	APN	B	205	1	21,21,22	0.65	0	27,28,30	0.97	3 (11%)
1	TPN	B	206	1	19,19,20	0.72	0	24,25,27	0.97	2 (8%)
1	APN	A	103[A]	1	21,21,22	0.61	0	27,28,30	0.97	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CPN	B	209[A]	1	18,18,19	0.54	0	21,23,25	1.07	1 (4%)
1	TPN	A	110	1	19,19,20	0.53	0	24,25,27	1.10	1 (4%)
1	GPN	B	204[A]	1	22,22,23	0.72	0	29,30,32	1.02	2 (6%)
1	APN	A	108[A]	1	21,21,22	0.80	1 (4%)	27,28,30	1.00	3 (11%)
1	TPN	A	106	1	19,19,20	0.76	1 (5%)	24,25,27	0.78	1 (4%)
1	CPN	A	107[A]	1	18,18,19	0.66	1 (5%)	21,23,25	1.05	2 (9%)
1	CPN	B	207[A]	1	18,18,19	0.66	0	21,23,25	1.10	3 (14%)
1	APN	B	203[A]	1	21,21,22	0.58	0	27,28,30	1.01	3 (11%)
1	TPN	B	210	1	19,19,20	0.79	1 (5%)	24,25,27	0.87	1 (4%)
1	CPN	A	109[A]	1	18,18,19	0.60	0	21,23,25	1.12	1 (4%)
1	APN	A	105	1	21,21,22	0.83	1 (4%)	27,28,30	0.99	2 (7%)
1	APN	A	103[B]	1	21,21,22	0.52	0	27,28,30	1.11	3 (11%)
1	GPN	A	104[A]	1	22,22,23	0.67	0	29,30,32	1.05	2 (6%)
1	APN	B	208[A]	1	21,21,22	0.51	0	27,28,30	0.94	3 (11%)
1	CPN	B	209[B]	1	18,18,19	0.64	0	21,23,25	1.02	1 (4%)
1	GPN	B	204[B]	1	22,22,23	0.72	0	29,30,32	1.03	2 (6%)
1	APN	A	108[B]	1	21,21,22	1.02	2 (9%)	27,28,30	1.54	3 (11%)
1	CPN	A	107[B]	1	18,18,19	0.45	0	21,23,25	1.12	2 (9%)
1	APN	B	203[B]	1	21,21,22	0.55	0	27,28,30	1.02	3 (11%)
1	CPN	B	207[B]	1	18,18,19	0.48	0	21,23,25	1.14	3 (14%)
1	CPN	A	109[B]	1	18,18,19	0.65	0	21,23,25	1.11	1 (4%)

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	104[B]	1	-	1/13/14/15	0/2/2/2
1	APN	B	208[B]	1	-	3/13/14/15	0/2/2/2
1	APN	B	205	1	-	1/13/14/15	0/2/2/2
1	TPN	B	206	1	-	0/13/14/15	0/1/1/1
1	APN	A	103[A]	1	-	9/13/14/15	0/2/2/2
1	CPN	B	209[A]	1	-	0/13/14/15	0/1/1/1
1	TPN	A	110	1	-	0/13/14/15	0/1/1/1
1	GPN	B	204[A]	1	-	1/13/14/15	0/2/2/2
1	APN	A	108[A]	1	-	7/13/14/15	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPN	A	106	1	-	0/13/14/15	0/1/1/1
1	CPN	A	107[A]	1	-	0/13/14/15	0/1/1/1
1	CPN	B	207[A]	1	-	0/13/14/15	0/1/1/1
1	APN	B	203[A]	1	-	8/13/14/15	0/2/2/2
1	TPN	B	210	1	-	2/13/14/15	0/1/1/1
1	CPN	A	109[A]	1	-	5/13/14/15	0/1/1/1
1	APN	A	105	1	-	0/13/14/15	0/2/2/2
1	APN	A	103[B]	1	-	4/13/14/15	0/2/2/2
1	GPN	A	104[A]	1	-	1/13/14/15	0/2/2/2
1	APN	B	208[A]	1	-	1/13/14/15	0/2/2/2
1	CPN	B	209[B]	1	-	1/13/14/15	0/1/1/1
1	GPN	B	204[B]	1	-	2/13/14/15	0/2/2/2
1	APN	A	108[B]	1	-	6/13/14/15	0/2/2/2
1	CPN	A	107[B]	1	-	0/13/14/15	0/1/1/1
1	APN	B	203[B]	1	-	6/13/14/15	0/2/2/2
1	CPN	B	207[B]	1	-	0/13/14/15	0/1/1/1
1	CPN	A	109[B]	1	-	3/13/14/15	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108[B]	APN	C5'-N4'	2.94	1.51	1.47
1	A	108[A]	APN	C8'-C7'	2.30	1.56	1.53
1	A	108[B]	APN	C8'-C7'	2.30	1.56	1.53
1	B	210	TPN	C5'-N4'	2.18	1.50	1.47
1	A	105	APN	C8'-N9	-2.13	1.43	1.46
1	A	106	TPN	C8'-N1	-2.13	1.43	1.46
1	A	107[A]	CPN	C5'-N4'	2.00	1.50	1.47

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108[B]	APN	C5'-N4'-C3'	-6.30	108.11	117.06
1	B	208[B]	APN	C5'-N4'-C3'	-4.79	110.26	117.06
1	A	110	TPN	C8'-C7'-N4'	3.73	121.56	117.04
1	A	104[A]	GPN	C8'-C7'-N4'	3.57	121.37	117.04
1	A	104[B]	GPN	C8'-C7'-N4'	3.57	121.37	117.04
1	A	103[B]	APN	C8'-N9-C8	3.17	130.41	127.27
1	B	203[B]	APN	C8'-C7'-N4'	3.16	120.87	117.04
1	B	208[A]	APN	C8'-C7'-N4'	3.16	120.87	117.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208[B]	APN	C8'-C7'-N4'	3.16	120.87	117.04
1	B	203[A]	APN	C8'-C7'-N4'	3.09	120.78	117.04
1	B	204[A]	GPN	C8'-C7'-N4'	3.04	120.72	117.04
1	B	204[B]	GPN	C8'-C7'-N4'	3.04	120.72	117.04
1	B	209[A]	CPN	C8'-C7'-N4'	2.98	120.66	117.04
1	B	209[B]	CPN	C8'-C7'-N4'	2.98	120.66	117.04
1	A	103[B]	APN	C8'-C7'-N4'	2.94	120.61	117.04
1	A	109[A]	CPN	C8'-C7'-N4'	2.91	120.57	117.04
1	A	109[B]	CPN	C8'-C7'-N4'	2.91	120.57	117.04
1	B	210	TPN	C8'-C7'-N4'	2.89	120.55	117.04
1	B	206	TPN	C8'-C7'-N4'	2.87	120.52	117.04
1	A	105	APN	C8'-C7'-N4'	2.84	120.49	117.04
1	B	207[A]	CPN	C8'-C7'-N4'	2.78	120.41	117.04
1	B	207[B]	CPN	C8'-C7'-N4'	2.78	120.41	117.04
1	A	103[A]	APN	C8'-N9-C8	2.75	130.00	127.27
1	A	107[A]	CPN	C8'-C7'-N4'	2.68	120.29	117.04
1	A	107[B]	CPN	C8'-C7'-N4'	2.68	120.29	117.04
1	A	103[A]	APN	C8'-C7'-N4'	2.63	120.23	117.04
1	B	205	APN	C8'-C7'-N4'	2.61	120.21	117.04
1	A	105	APN	C8'-N9-C8	2.60	129.85	127.27
1	A	108[A]	APN	C8'-N9-C8	2.55	129.80	127.27
1	A	108[B]	APN	C8'-N9-C8	2.55	129.80	127.27
1	B	205	APN	C8'-N9-C8	2.46	129.71	127.27
1	B	203[A]	APN	C8'-N9-C8	2.44	129.68	127.27
1	B	203[B]	APN	C8'-N9-C8	2.41	129.66	127.27
1	A	108[A]	APN	C5'-N4'-C3'	-2.40	113.64	117.06
1	B	207[A]	CPN	C7'-C8'-N1	2.36	113.92	110.73
1	B	207[B]	CPN	C7'-C8'-N1	2.36	113.92	110.73
1	A	106	TPN	C8'-C7'-N4'	2.32	119.85	117.04
1	B	208[B]	APN	C2'-C3'-N4'	-2.29	107.77	112.91
1	A	107[A]	CPN	C7'-C8'-N1	2.28	113.81	110.73
1	A	107[B]	CPN	C7'-C8'-N1	2.28	113.81	110.73
1	A	104[A]	GPN	O7'-C7'-N4'	-2.25	118.12	122.12
1	A	104[B]	GPN	O7'-C7'-N4'	-2.25	118.12	122.12
1	A	108[A]	APN	C7'-C8'-N9	2.23	113.72	110.81
1	A	108[B]	APN	C7'-C8'-N9	2.23	113.72	110.81
1	B	206	TPN	O7'-C7'-N4'	-2.22	118.17	122.12
1	B	205	APN	O7'-C7'-N4'	-2.15	118.30	122.12
1	B	203[A]	APN	O7'-C7'-N4'	-2.12	118.35	122.12
1	B	207[A]	CPN	O7'-C7'-N4'	-2.09	118.40	122.12
1	B	207[B]	CPN	O7'-C7'-N4'	-2.09	118.40	122.12
1	B	208[A]	APN	O7'-C7'-N4'	-2.08	118.41	122.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208[B]	APN	O7'-C7'-N4'	-2.08	118.41	122.12
1	B	204[A]	GPN	C8'-N9-C4	-2.08	124.17	127.02
1	B	204[B]	GPN	C8'-N9-C4	-2.08	124.17	127.02
1	B	208[A]	APN	C8'-N9-C8	2.07	129.32	127.27
1	B	208[B]	APN	C8'-N9-C8	2.07	129.32	127.27
1	B	208[B]	APN	C3'-N4'-C7'	2.06	128.26	121.06
1	B	203[B]	APN	O7'-C7'-N4'	-2.05	118.46	122.12
1	A	103[B]	APN	O7'-C7'-N4'	-2.03	118.51	122.12

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	103[A]	APN	C8'-C7'-N4'-C5'
1	A	103[A]	APN	C8'-C7'-N4'-C3'
1	A	103[A]	APN	O7'-C7'-N4'-C5'
1	A	103[A]	APN	C2'-C3'-N4'-C7'
1	A	103[B]	APN	C7'-C8'-N9-C8
1	A	103[B]	APN	C7'-C8'-N9-C4
1	A	103[B]	APN	C-C5'-N4'-C7'
1	A	108[A]	APN	C8'-C7'-N4'-C5'
1	A	108[A]	APN	O7'-C7'-N4'-C5'
1	A	108[A]	APN	C-C5'-N4'-C7'
1	A	108[A]	APN	N-C2'-C3'-N4'
1	A	108[B]	APN	C-C5'-N4'-C7'
1	A	109[A]	CPN	N-C2'-C3'-N4'
1	B	203[A]	APN	C7'-C8'-N9-C8
1	B	203[A]	APN	C2'-C3'-N4'-C7'
1	B	203[B]	APN	C8'-C7'-N4'-C5'
1	B	203[B]	APN	C8'-C7'-N4'-C3'
1	B	203[B]	APN	O7'-C7'-N4'-C5'
1	B	203[B]	APN	O7'-C7'-N4'-C3'
1	B	203[B]	APN	N-C2'-C3'-N4'
1	B	204[B]	GPN	N-C2'-C3'-N4'
1	B	208[B]	APN	C-C5'-N4'-C7'
1	B	210	TPN	C-C5'-N4'-C7'
1	A	103[A]	APN	O7'-C7'-N4'-C3'
1	A	108[B]	APN	C8'-C7'-N4'-C3'
1	A	108[B]	APN	O7'-C7'-N4'-C3'
1	B	203[A]	APN	O7'-C7'-N4'-C5'
1	B	208[B]	APN	C2'-C3'-N4'-C5'
1	A	108[B]	APN	O7'-C7'-N4'-C5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	B	203[A]	APN	C8'-C7'-N4'-C5'
1	A	108[A]	APN	O7'-C7'-N4'-C3'
1	B	204[B]	GPN	C2'-C3'-N4'-C5'
1	A	108[B]	APN	C8'-C7'-N4'-C5'
1	B	203[A]	APN	O7'-C7'-N4'-C3'
1	A	103[A]	APN	N-C2'-C3'-N4'
1	A	103[B]	APN	N-C2'-C3'-N4'
1	A	104[A]	GPN	N-C2'-C3'-N4'
1	A	104[B]	GPN	N-C2'-C3'-N4'
1	A	109[B]	CPN	N-C2'-C3'-N4'
1	B	203[A]	APN	N-C2'-C3'-N4'
1	B	204[A]	GPN	N-C2'-C3'-N4'
1	B	209[B]	CPN	N-C2'-C3'-N4'
1	A	109[A]	CPN	O7'-C7'-N4'-C5'
1	A	109[B]	CPN	O7'-C7'-N4'-C5'
1	A	108[A]	APN	C8'-C7'-N4'-C3'
1	A	109[A]	CPN	O7'-C7'-N4'-C3'
1	A	108[A]	APN	C-C5'-N4'-C3'
1	A	108[B]	APN	C-C5'-N4'-C3'
1	A	109[A]	CPN	C8'-C7'-N4'-C5'
1	A	109[B]	CPN	C8'-C7'-N4'-C5'
1	A	103[A]	APN	C2'-C3'-N4'-C5'
1	A	103[A]	APN	C-C5'-N4'-C7'
1	B	205	APN	C-C5'-N4'-C7'
1	B	208[A]	APN	C-C5'-N4'-C7'
1	A	109[A]	CPN	C8'-C7'-N4'-C3'
1	B	203[A]	APN	C8'-C7'-N4'-C3'
1	B	208[B]	APN	C-C5'-N4'-C3'
1	B	210	TPN	C-C5'-N4'-C3'
1	B	203[A]	APN	C2'-C3'-N4'-C5'
1	A	103[A]	APN	C7'-C8'-N9-C8
1	B	203[B]	APN	C7'-C8'-N9-C8

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	208[B]	APN	1	0
1	A	108[A]	APN	1	0
1	B	203[A]	APN	1	0
1	B	210	TPN	2	0
1	A	108[B]	APN	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	107[B]	CPN	2	0
1	B	207[B]	CPN	1	0
1	A	109[B]	CPN	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 28 such residues modelled in this entry, 2 are modelled with single atom - leaving 26 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	104[B]	1	22,22,23	0.67	0	29,30,32	1.06	2 (6%)
1	APN	B	208[B]	1	21,21,22	0.65	0	27,28,30	1.43	6 (22%)
1	APN	B	205	1	21,21,22	0.65	0	27,28,30	0.97	3 (11%)
1	TPN	B	206	1	19,19,20	0.72	0	24,25,27	0.97	2 (8%)
1	APN	A	103[A]	1	21,21,22	0.61	0	27,28,30	0.97	2 (7%)
1	CPN	B	209[A]	1	18,18,19	0.54	0	21,23,25	1.07	1 (4%)
1	TPN	A	110	1	19,19,20	0.53	0	24,25,27	1.10	1 (4%)
1	GPN	B	204[A]	1	22,22,23	0.72	0	29,30,32	1.02	2 (6%)
1	APN	A	108[A]	1	21,21,22	0.80	1 (4%)	27,28,30	1.00	3 (11%)
1	TPN	A	106	1	19,19,20	0.76	1 (5%)	24,25,27	0.78	1 (4%)
1	CPN	A	107[A]	1	18,18,19	0.66	1 (5%)	21,23,25	1.05	2 (9%)
1	CPN	B	207[A]	1	18,18,19	0.66	0	21,23,25	1.10	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	APN	B	203[A]	1	21,21,22	0.58	0	27,28,30	1.01	3 (11%)
1	TPN	B	210	1	19,19,20	0.79	1 (5%)	24,25,27	0.87	1 (4%)
1	CPN	A	109[A]	1	18,18,19	0.60	0	21,23,25	1.12	1 (4%)
1	APN	A	105	1	21,21,22	0.83	1 (4%)	27,28,30	0.99	2 (7%)
1	APN	A	103[B]	1	21,21,22	0.52	0	27,28,30	1.11	3 (11%)
1	GPN	A	104[A]	1	22,22,23	0.67	0	29,30,32	1.05	2 (6%)
1	APN	B	208[A]	1	21,21,22	0.51	0	27,28,30	0.94	3 (11%)
1	CPN	B	209[B]	1	18,18,19	0.64	0	21,23,25	1.02	1 (4%)
1	GPN	B	204[B]	1	22,22,23	0.72	0	29,30,32	1.03	2 (6%)
1	APN	A	108[B]	1	21,21,22	1.02	2 (9%)	27,28,30	1.54	3 (11%)
1	CPN	A	107[B]	1	18,18,19	0.45	0	21,23,25	1.12	2 (9%)
1	APN	B	203[B]	1	21,21,22	0.55	0	27,28,30	1.02	3 (11%)
1	CPN	B	207[B]	1	18,18,19	0.48	0	21,23,25	1.14	3 (14%)
1	CPN	A	109[B]	1	18,18,19	0.65	0	21,23,25	1.11	1 (4%)

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	104[B]	1	-	1/13/14/15	0/2/2/2
1	APN	B	208[B]	1	-	3/13/14/15	0/2/2/2
1	APN	B	205	1	-	1/13/14/15	0/2/2/2
1	TPN	B	206	1	-	0/13/14/15	0/1/1/1
1	APN	A	103[A]	1	-	9/13/14/15	0/2/2/2
1	CPN	B	209[A]	1	-	0/13/14/15	0/1/1/1
1	TPN	A	110	1	-	0/13/14/15	0/1/1/1
1	GPN	B	204[A]	1	-	1/13/14/15	0/2/2/2
1	APN	A	108[A]	1	-	7/13/14/15	0/2/2/2
1	TPN	A	106	1	-	0/13/14/15	0/1/1/1
1	CPN	A	107[A]	1	-	0/13/14/15	0/1/1/1
1	CPN	B	207[A]	1	-	0/13/14/15	0/1/1/1
1	APN	B	203[A]	1	-	8/13/14/15	0/2/2/2
1	TPN	B	210	1	-	2/13/14/15	0/1/1/1
1	CPN	A	109[A]	1	-	5/13/14/15	0/1/1/1
1	APN	A	105	1	-	0/13/14/15	0/2/2/2
1	APN	A	103[B]	1	-	4/13/14/15	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GPN	A	104[A]	1	-	1/13/14/15	0/2/2/2
1	APN	B	208[A]	1	-	1/13/14/15	0/2/2/2
1	CPN	B	209[B]	1	-	1/13/14/15	0/1/1/1
1	GPN	B	204[B]	1	-	2/13/14/15	0/2/2/2
1	APN	A	108[B]	1	-	6/13/14/15	0/2/2/2
1	CPN	A	107[B]	1	-	0/13/14/15	0/1/1/1
1	APN	B	203[B]	1	-	6/13/14/15	0/2/2/2
1	CPN	B	207[B]	1	-	0/13/14/15	0/1/1/1
1	CPN	A	109[B]	1	-	3/13/14/15	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108[B]	APN	C5'-N4'	2.94	1.51	1.47
1	A	108[A]	APN	C8'-C7'	2.30	1.56	1.53
1	A	108[B]	APN	C8'-C7'	2.30	1.56	1.53
1	B	210	TPN	C5'-N4'	2.18	1.50	1.47
1	A	105	APN	C8'-N9	-2.13	1.43	1.46
1	A	106	TPN	C8'-N1	-2.13	1.43	1.46
1	A	107[A]	CPN	C5'-N4'	2.00	1.50	1.47

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108[B]	APN	C5'-N4'-C3'	-6.30	108.11	117.06
1	B	208[B]	APN	C5'-N4'-C3'	-4.79	110.26	117.06
1	A	110	TPN	C8'-C7'-N4'	3.73	121.56	117.04
1	A	104[A]	GPN	C8'-C7'-N4'	3.57	121.37	117.04
1	A	104[B]	GPN	C8'-C7'-N4'	3.57	121.37	117.04
1	A	103[B]	APN	C8'-N9-C8	3.17	130.41	127.27
1	B	203[B]	APN	C8'-C7'-N4'	3.16	120.87	117.04
1	B	208[A]	APN	C8'-C7'-N4'	3.16	120.87	117.04
1	B	208[B]	APN	C8'-C7'-N4'	3.16	120.87	117.04
1	B	203[A]	APN	C8'-C7'-N4'	3.09	120.78	117.04
1	B	204[A]	GPN	C8'-C7'-N4'	3.04	120.72	117.04
1	B	204[B]	GPN	C8'-C7'-N4'	3.04	120.72	117.04
1	B	209[A]	CPN	C8'-C7'-N4'	2.98	120.66	117.04
1	B	209[B]	CPN	C8'-C7'-N4'	2.98	120.66	117.04
1	A	103[B]	APN	C8'-C7'-N4'	2.94	120.61	117.04
1	A	109[A]	CPN	C8'-C7'-N4'	2.91	120.57	117.04
1	A	109[B]	CPN	C8'-C7'-N4'	2.91	120.57	117.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	TPN	C8'-C7'-N4'	2.89	120.55	117.04
1	B	206	TPN	C8'-C7'-N4'	2.87	120.52	117.04
1	A	105	APN	C8'-C7'-N4'	2.84	120.49	117.04
1	B	207[A]	CPN	C8'-C7'-N4'	2.78	120.41	117.04
1	B	207[B]	CPN	C8'-C7'-N4'	2.78	120.41	117.04
1	A	103[A]	APN	C8'-N9-C8	2.75	130.00	127.27
1	A	107[A]	CPN	C8'-C7'-N4'	2.68	120.29	117.04
1	A	107[B]	CPN	C8'-C7'-N4'	2.68	120.29	117.04
1	A	103[A]	APN	C8'-C7'-N4'	2.63	120.23	117.04
1	B	205	APN	C8'-C7'-N4'	2.61	120.21	117.04
1	A	105	APN	C8'-N9-C8	2.60	129.85	127.27
1	A	108[A]	APN	C8'-N9-C8	2.55	129.80	127.27
1	A	108[B]	APN	C8'-N9-C8	2.55	129.80	127.27
1	B	205	APN	C8'-N9-C8	2.46	129.71	127.27
1	B	203[A]	APN	C8'-N9-C8	2.44	129.68	127.27
1	B	203[B]	APN	C8'-N9-C8	2.41	129.66	127.27
1	A	108[A]	APN	C5'-N4'-C3'	-2.40	113.64	117.06
1	B	207[A]	CPN	C7'-C8'-N1	2.36	113.92	110.73
1	B	207[B]	CPN	C7'-C8'-N1	2.36	113.92	110.73
1	A	106	TPN	C8'-C7'-N4'	2.32	119.85	117.04
1	B	208[B]	APN	C2'-C3'-N4'	-2.29	107.77	112.91
1	A	107[A]	CPN	C7'-C8'-N1	2.28	113.81	110.73
1	A	107[B]	CPN	C7'-C8'-N1	2.28	113.81	110.73
1	A	104[A]	GPN	O7'-C7'-N4'	-2.25	118.12	122.12
1	A	104[B]	GPN	O7'-C7'-N4'	-2.25	118.12	122.12
1	A	108[A]	APN	C7'-C8'-N9	2.23	113.72	110.81
1	A	108[B]	APN	C7'-C8'-N9	2.23	113.72	110.81
1	B	206	TPN	O7'-C7'-N4'	-2.22	118.17	122.12
1	B	205	APN	O7'-C7'-N4'	-2.15	118.30	122.12
1	B	203[A]	APN	O7'-C7'-N4'	-2.12	118.35	122.12
1	B	207[A]	CPN	O7'-C7'-N4'	-2.09	118.40	122.12
1	B	207[B]	CPN	O7'-C7'-N4'	-2.09	118.40	122.12
1	B	208[A]	APN	O7'-C7'-N4'	-2.08	118.41	122.12
1	B	208[B]	APN	O7'-C7'-N4'	-2.08	118.41	122.12
1	B	204[A]	GPN	C8'-N9-C4	-2.08	124.17	127.02
1	B	204[B]	GPN	C8'-N9-C4	-2.08	124.17	127.02
1	B	208[A]	APN	C8'-N9-C8	2.07	129.32	127.27
1	B	208[B]	APN	C8'-N9-C8	2.07	129.32	127.27
1	B	208[B]	APN	C3'-N4'-C7'	2.06	128.26	121.06
1	B	203[B]	APN	O7'-C7'-N4'	-2.05	118.46	122.12
1	A	103[B]	APN	O7'-C7'-N4'	-2.03	118.51	122.12

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	103[A]	APN	C8'-C7'-N4'-C5'
1	A	103[A]	APN	C8'-C7'-N4'-C3'
1	A	103[A]	APN	O7'-C7'-N4'-C5'
1	A	103[A]	APN	C2'-C3'-N4'-C7'
1	A	103[B]	APN	C7'-C8'-N9-C8
1	A	103[B]	APN	C7'-C8'-N9-C4
1	A	103[B]	APN	C-C5'-N4'-C7'
1	A	108[A]	APN	C8'-C7'-N4'-C5'
1	A	108[A]	APN	O7'-C7'-N4'-C5'
1	A	108[A]	APN	C-C5'-N4'-C7'
1	A	108[A]	APN	N-C2'-C3'-N4'
1	A	108[B]	APN	C-C5'-N4'-C7'
1	A	109[A]	CPN	N-C2'-C3'-N4'
1	B	203[A]	APN	C7'-C8'-N9-C8
1	B	203[A]	APN	C2'-C3'-N4'-C7'
1	B	203[B]	APN	C8'-C7'-N4'-C5'
1	B	203[B]	APN	C8'-C7'-N4'-C3'
1	B	203[B]	APN	O7'-C7'-N4'-C5'
1	B	203[B]	APN	O7'-C7'-N4'-C3'
1	B	203[B]	APN	N-C2'-C3'-N4'
1	B	204[B]	GPN	N-C2'-C3'-N4'
1	B	208[B]	APN	C-C5'-N4'-C7'
1	B	210	TPN	C-C5'-N4'-C7'
1	A	103[A]	APN	O7'-C7'-N4'-C3'
1	A	108[B]	APN	C8'-C7'-N4'-C3'
1	A	108[B]	APN	O7'-C7'-N4'-C3'
1	B	203[A]	APN	O7'-C7'-N4'-C5'
1	B	208[B]	APN	C2'-C3'-N4'-C5'
1	A	108[B]	APN	O7'-C7'-N4'-C5'
1	B	203[A]	APN	C8'-C7'-N4'-C5'
1	A	108[A]	APN	O7'-C7'-N4'-C3'
1	B	204[B]	GPN	C2'-C3'-N4'-C5'
1	A	108[B]	APN	C8'-C7'-N4'-C5'
1	B	203[A]	APN	O7'-C7'-N4'-C3'
1	A	103[A]	APN	N-C2'-C3'-N4'
1	A	103[B]	APN	N-C2'-C3'-N4'
1	A	104[A]	GPN	N-C2'-C3'-N4'
1	A	104[B]	GPN	N-C2'-C3'-N4'
1	A	109[B]	CPN	N-C2'-C3'-N4'
1	B	203[A]	APN	N-C2'-C3'-N4'
1	B	204[A]	GPN	N-C2'-C3'-N4'
1	B	209[B]	CPN	N-C2'-C3'-N4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	109[A]	CPN	O7'-C7'-N4'-C5'
1	A	109[B]	CPN	O7'-C7'-N4'-C5'
1	A	108[A]	APN	C8'-C7'-N4'-C3'
1	A	109[A]	CPN	O7'-C7'-N4'-C3'
1	A	108[A]	APN	C-C5'-N4'-C3'
1	A	108[B]	APN	C-C5'-N4'-C3'
1	A	109[A]	CPN	C8'-C7'-N4'-C5'
1	A	109[B]	CPN	C8'-C7'-N4'-C5'
1	A	103[A]	APN	C2'-C3'-N4'-C5'
1	A	103[A]	APN	C-C5'-N4'-C7'
1	B	205	APN	C-C5'-N4'-C7'
1	B	208[A]	APN	C-C5'-N4'-C7'
1	A	109[A]	CPN	C8'-C7'-N4'-C3'
1	B	203[A]	APN	C8'-C7'-N4'-C3'
1	B	208[B]	APN	C-C5'-N4'-C3'
1	B	210	TPN	C-C5'-N4'-C3'
1	B	203[A]	APN	C2'-C3'-N4'-C5'
1	A	103[A]	APN	C7'-C8'-N9-C8
1	B	203[B]	APN	C7'-C8'-N9-C8

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	208[B]	APN	1	0
1	A	108[A]	APN	1	0
1	B	203[A]	APN	1	0
1	B	210	TPN	2	0
1	A	108[B]	APN	1	0
1	A	107[B]	CPN	2	0
1	B	207[B]	CPN	1	0
1	A	109[B]	CPN	1	0

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

There are no RSRZ outliers to report within protein, DNA, RNA chains in this entry.

5.2 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	APN	B	203[A]	20/21	0.72	0.27	39,44,45,47	20
1	APN	B	203[B]	20/21	0.72	0.27	39,41,43,44	20
1	APN	A	103[A]	20/21	0.77	0.23	37,39,44,45	20
1	APN	A	103[B]	20/21	0.77	0.23	37,40,43,43	20
1	TPN	B	210	19/20	0.82	0.16	39,46,56,57	0
1	TPN	A	110	19/20	0.84	0.18	42,48,58,60	0
1	APN	A	108[A]	20/21	0.85	0.17	38,44,46,46	6
1	APN	A	108[B]	20/21	0.85	0.17	41,44,47,49	6
1	GPN	B	204[B]	21/22	0.86	0.15	41,43,45,46	2
1	GPN	B	204[A]	21/22	0.86	0.15	41,43,45,46	2
1	TPN	A	106	19/20	0.88	0.14	31,33,35,35	0
1	CPN	A	107[A]	18/19	0.89	0.14	31,36,42,42	3
1	CPN	A	107[B]	18/19	0.89	0.14	31,40,42,42	3
1	GPN	A	104[B]	21/22	0.89	0.14	40,42,44,47	2
1	GPN	A	104[A]	21/22	0.89	0.14	38,42,44,47	2
1	CPN	A	109[A]	18/19	0.89	0.14	45,49,52,52	3
1	CPN	B	207[A]	18/19	0.89	0.12	30,34,40,41	3
1	CPN	B	207[B]	18/19	0.89	0.12	30,38,40,41	3
1	CPN	B	209[A]	18/19	0.89	0.15	35,42,50,52	3
1	CPN	B	209[B]	18/19	0.89	0.15	35,42,50,52	3
1	CPN	A	109[B]	18/19	0.89	0.14	45,49,52,52	3
1	APN	B	208[B]	20/21	0.90	0.14	40,46,47,48	6
1	APN	A	105	20/21	0.90	0.14	28,37,40,42	0
1	TPN	B	206	19/20	0.90	0.12	30,33,36,37	0
1	APN	B	208[A]	20/21	0.90	0.14	37,44,47,48	6
1	APN	B	205	20/21	0.91	0.13	30,35,43,44	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.