



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:49 PM UTC

PDB ID : 3MBU / pdb_00003mbu
Title : Structure of a bipyridine-modified PNA duplex
Authors : Yeh, J.I.; Pohl, E.; Truan, D.; He, W.; Sheldrick, G.M.; Du, S.; Achim, C.
Deposited on : 2010-03-26
Resolution : 1.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

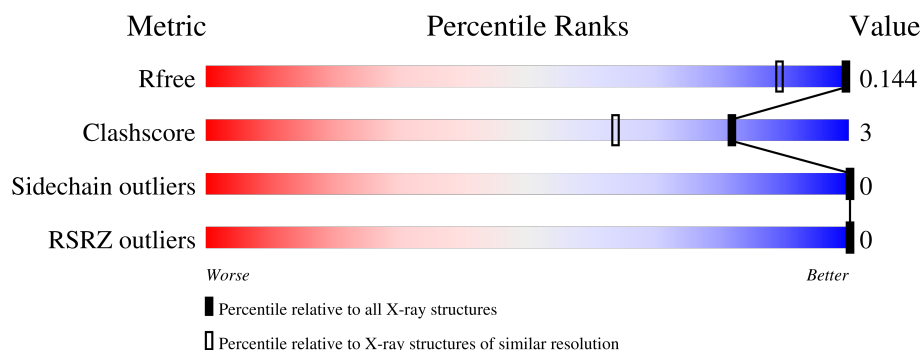
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.05 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	1182 (1.08-1.04)
Clashscore	190562	1204 (1.08-1.04)
Sidechain outliers	187428	1176 (1.08-1.04)
RSRZ outliers	180081	1181 (1.08-1.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	10	10%90%
1	B	10	20%80%
1	C	10	20%80%
1	D	10	10%80%10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	D	5010	-	X	-	-

2 Entry composition [i](#)

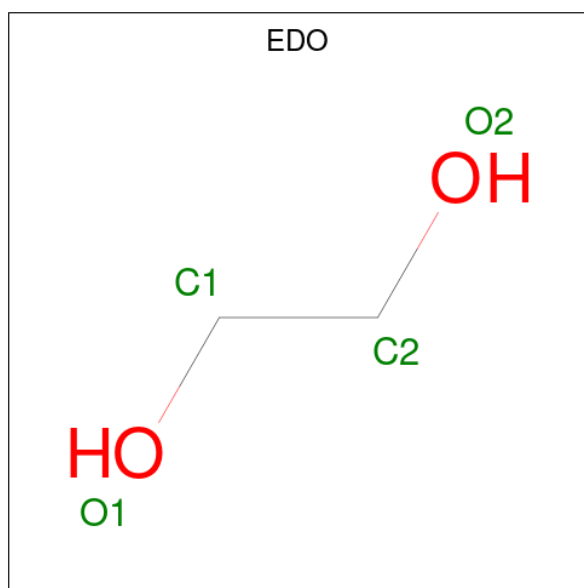
There are 7 unique types of molecules in this entry. The entry contains 1021 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Bipyridine-PNA.

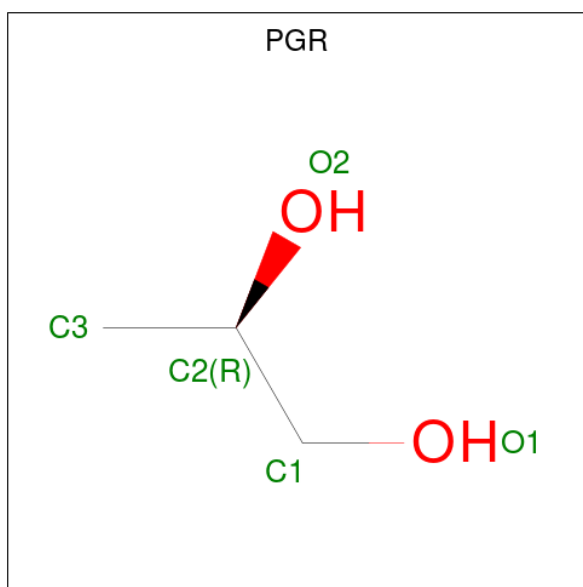
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	10	Total	C	N	O	0	0	0
			183	104	52	27			
1	B	10	Total	C	N	O	0	0	0
			183	104	52	27			
1	C	10	Total	C	N	O	0	0	0
			187	107	53	27			
1	D	10	Total	C	N	O	0	0	0
			187	107	53	27			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



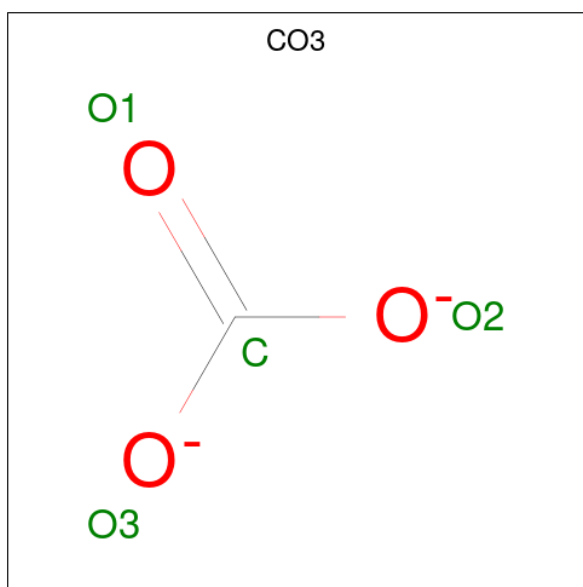
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is R-1,2-PROPANEDIOL (CCD ID: PGR) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 4 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	1	3		

Continued on next page...

Continued from previous page...

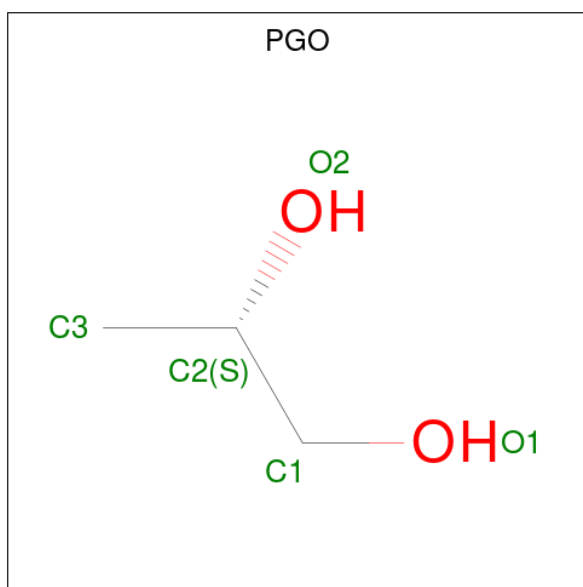
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			5	3	2		
6	D	1	Total	C	O	0	0
			5	3	2		

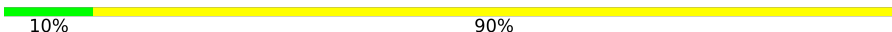
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	62	Total	O	0	0
			62	62		
7	B	49	Total	O	0	0
			49	49		
7	C	62	Total	O	0	0
			62	62		
7	D	59	Total	O	0	0
			59	59		

3 Residue-property plots [i](#)

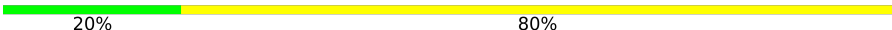
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Bipyridine-PNA

Chain A: 

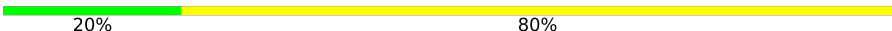
GPN1001
GPN1002
CPN1003
APN1004
KPN1005
TPN1006
GPN1007
CPN1008
CPN1009
K1010

- Molecule 1: Bipyridine-PNA

Chain B: 

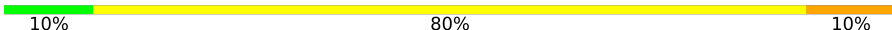
GPN2001
GPN2002
CPN2003
APN2004
KPN2005
TPN2006
GPN2007
CPN2008
CPN2009
K2010

- Molecule 1: Bipyridine-PNA

Chain C: 

GPN3001
GPN3002
CPN3003
APN3004
KPN3005
TPN3006
GPN3007
CPN3008
CPN3009
K3010

- Molecule 1: Bipyridine-PNA

Chain D: 

GPN4001
GPN4002
CPN4003
APN4004
KPN4005
TPN4006
GPN4007
CPN4008
CPN4009
K4010

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	38.20Å 25.73Å 53.05Å 90.00° 105.33° 90.00°	Depositor
Resolution (Å)	26.73 – 1.05 26.73 – 1.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (26.73-1.05) 90.9 (26.73-1.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 1.10Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.127 , 0.169 (Not available) , 0.144	Depositor DCC
R_{free} test set	1930 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	8.3	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1021	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2253e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

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, CO3, CPN, GPN, PGO, APN, KPN, PGR, EDO, GOL

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	0.37	0/4	1.55	0/4
1	B	0.71	0/4	1.18	0/4
1	C	0.76	0/8	0.96	0/8
1	D	0.45	0/8	1.24	0/8
All	All	0.61	0/24	1.21	0/24

There are no bond length outliers.

There are no bond angle outliers.

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	183	0	78	0	0
1	B	183	0	78	0	0
1	C	187	0	89	0	0
1	D	187	0	89	3	0
2	A	4	0	6	0	0
3	A	5	0	8	0	0
3	B	10	0	16	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	6	0	8	0	0
5	D	6	0	6	3	0
6	C	5	0	8	0	0
6	D	5	0	8	0	0
7	A	62	0	0	0	0
7	B	49	0	0	0	0
7	C	62	0	0	0	0
7	D	59	0	0	0	0
All	All	1021	0	394	3	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 3.

All (3) 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:D:4002:GPN:HN22	5:D:5010:GOL:H32	1.28	0.97
1:D:4002:GPN:N2	5:D:5010:GOL:H32	2.07	0.66
1:D:4002:GPN:HN22	5:D:5010:GOL:C3	2.14	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	1/1 (100%)	1 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	1/1 (100%)	1 (100%)	0	100	100
All	All	2/2 (100%)	2 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	GPN	C	3007	1	22,22,23	0.87	1 (4%)	29,30,32	1.01	1 (3%)
1	GPN	D	4001	1	22,22,23	1.04	1 (4%)	29,30,32	1.20	4 (13%)
1	CPN	A	1008	1	18,18,19	0.75	0	21,23,25	1.17	1 (4%)
1	KPN	B	2005	1	23,23,24	1.13	2 (8%)	28,29,31	2.39	12 (42%)
1	TPN	C	3006	1	19,19,20	0.83	0	24,25,27	1.17	1 (4%)
1	GPN	D	4002	1	22,22,23	0.88	1 (4%)	29,30,32	0.93	1 (3%)
1	CPN	A	1003	1	18,18,19	0.75	0	21,23,25	1.12	1 (4%)
1	GPN	C	3001	1	22,22,23	0.56	0	29,30,32	0.72	0
1	CPN	D	4009	1	18,18,19	0.82	0	21,23,25	1.00	2 (9%)
1	CPN	B	2008	1	18,18,19	0.77	0	21,23,25	0.90	0
1	GPN	A	1007	1	22,22,23	0.95	1 (4%)	29,30,32	1.09	1 (3%)
1	APN	D	4004	1	21,21,22	1.03	1 (4%)	27,28,30	1.07	1 (3%)
1	CPN	D	4008	1	18,18,19	0.66	0	21,23,25	1.19	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GPN	C	3002	1	22,22,23	0.83	1 (4%)	29,30,32	1.24	4 (13%)
1	CPN	C	3009	1	18,18,19	0.76	1 (5%)	21,23,25	0.91	1 (4%)
1	GPN	A	1002	1	22,22,23	0.89	1 (4%)	29,30,32	0.87	0
1	CPN	B	2003	1	18,18,19	0.72	0	21,23,25	0.90	2 (9%)
1	APN	A	1004	1	21,21,22	1.22	2 (9%)	27,28,30	1.28	4 (14%)
1	KPN	C	3005	1	23,23,24	1.28	1 (4%)	28,29,31	1.99	8 (28%)
1	KPN	A	1005	1	23,23,24	1.16	1 (4%)	28,29,31	2.06	9 (32%)
1	GPN	B	2002	1	22,22,23	0.88	0	29,30,32	0.83	1 (3%)
1	TPN	D	4006	1	19,19,20	1.23	1 (5%)	24,25,27	1.31	3 (12%)
1	CPN	C	3008	1	18,18,19	0.93	1 (5%)	21,23,25	0.96	1 (4%)
1	KPN	D	4005	1	23,23,24	1.05	1 (4%)	28,29,31	2.00	10 (35%)
1	GPN	D	4007	1	22,22,23	0.90	1 (4%)	29,30,32	1.02	3 (10%)
1	GPN	B	2007	1	22,22,23	0.89	1 (4%)	29,30,32	1.28	3 (10%)
1	GPN	A	1001	1	22,22,23	0.93	1 (4%)	29,30,32	0.90	0
1	TPN	A	1006	1	19,19,20	1.15	1 (5%)	24,25,27	1.48	4 (16%)
1	CPN	D	4003	1	18,18,19	0.91	1 (5%)	21,23,25	1.17	2 (9%)
1	CPN	A	1009	1	18,18,19	1.07	1 (5%)	21,23,25	1.07	1 (4%)
1	APN	C	3004	1	21,21,22	1.10	2 (9%)	27,28,30	1.55	5 (18%)
1	GPN	B	2001	1	22,22,23	0.92	0	29,30,32	1.13	2 (6%)
1	TPN	B	2006	1	19,19,20	1.43	4 (21%)	24,25,27	1.86	9 (37%)
1	CPN	B	2009	1	18,18,19	1.05	1 (5%)	21,23,25	1.13	1 (4%)
1	APN	B	2004	1	21,21,22	1.33	3 (14%)	27,28,30	2.21	7 (25%)
1	CPN	C	3003	1	18,18,19	0.83	0	21,23,25	0.85	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	C	3007	1	-	0/13/14/15	0/2/2/2
1	GPN	D	4001	1	-	0/13/14/15	0/2/2/2
1	CPN	A	1008	1	-	0/13/14/15	0/1/1/1
1	KPN	B	2005	1	-	6/17/18/19	0/2/2/2
1	TPN	C	3006	1	-	0/13/14/15	0/1/1/1
1	GPN	D	4002	1	-	0/13/14/15	0/2/2/2
1	CPN	A	1003	1	-	0/13/14/15	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GPN	C	3001	1	-	0/13/14/15	0/2/2/2
1	CPN	D	4009	1	-	0/13/14/15	0/1/1/1
1	CPN	B	2008	1	-	0/13/14/15	0/1/1/1
1	GPN	A	1007	1	-	0/13/14/15	0/2/2/2
1	APN	D	4004	1	-	0/13/14/15	0/2/2/2
1	CPN	D	4008	1	-	0/13/14/15	0/1/1/1
1	GPN	C	3002	1	-	0/13/14/15	0/2/2/2
1	CPN	C	3009	1	-	0/13/14/15	0/1/1/1
1	GPN	A	1002	1	-	0/13/14/15	0/2/2/2
1	CPN	B	2003	1	-	0/13/14/15	0/1/1/1
1	APN	A	1004	1	-	0/13/14/15	0/2/2/2
1	KPN	C	3005	1	-	1/17/18/19	0/2/2/2
1	KPN	A	1005	1	-	4/17/18/19	0/2/2/2
1	GPN	B	2002	1	-	0/13/14/15	0/2/2/2
1	TPN	D	4006	1	-	0/13/14/15	0/1/1/1
1	CPN	C	3008	1	-	0/13/14/15	0/1/1/1
1	KPN	D	4005	1	-	2/17/18/19	0/2/2/2
1	GPN	D	4007	1	-	0/13/14/15	0/2/2/2
1	GPN	B	2007	1	-	0/13/14/15	0/2/2/2
1	GPN	A	1001	1	-	1/13/14/15	0/2/2/2
1	TPN	A	1006	1	-	0/13/14/15	0/1/1/1
1	CPN	D	4003	1	-	0/13/14/15	0/1/1/1
1	CPN	A	1009	1	-	0/13/14/15	0/1/1/1
1	APN	C	3004	1	-	0/13/14/15	0/2/2/2
1	GPN	B	2001	1	-	0/13/14/15	0/2/2/2
1	TPN	B	2006	1	-	0/13/14/15	0/1/1/1
1	CPN	B	2009	1	-	0/13/14/15	0/1/1/1
1	APN	B	2004	1	-	0/13/14/15	0/2/2/2
1	CPN	C	3003	1	-	0/13/14/15	0/1/1/1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3005	KPN	C6-C5	-4.63	1.38	1.49
1	D	4005	KPN	C6-C5	-3.80	1.40	1.49
1	A	1005	KPN	C6-C5	-3.79	1.40	1.49
1	D	4001	GPN	C8-N9	-3.75	1.30	1.36
1	B	2006	TPN	C4-C5	-3.52	1.39	1.44

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2005	KPN	C10-N2-C6	6.12	125.81	117.24
1	B	2004	APN	C4-N9-C8	5.34	109.59	105.75
1	D	4005	KPN	C10-N2-C6	4.93	124.14	117.24
1	B	2004	APN	N9-C8-N7	-4.58	109.93	114.16
1	C	3005	KPN	C10-N2-C6	4.50	123.54	117.24

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	2005	KPN	C-C5'-N4'-C7'
1	A	1001	GPN	C2'-C3'-N4'-C5'
1	A	1005	KPN	N4'-C7'-C8'-C2
1	C	3005	KPN	N4'-C7'-C8'-C2
1	D	4005	KPN	N4'-C7'-C8'-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	4002	GPN	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	0.36	0	2,2,2	0.10	0
3	PGR	B	5005	-	4,4,4	1.10	0	4,4,4	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CO3	C	5002	-	3,3,3	2.40	1 (33%)	2,3,3	0.24	0
6	PGO	C	5007	-	4,4,4	0.85	0	4,4,4	0.86	0
5	GOL	C	5006	-	5,5,5	0.57	0	5,5,5	0.95	0
3	PGR	B	5004	-	4,4,4	0.59	0	4,4,4	0.95	0
3	PGR	A	5009	-	4,4,4	0.77	0	4,4,4	0.64	0
4	CO3	D	5001	-	3,3,3	2.71	1 (33%)	2,3,3	0.30	0
5	GOL	D	5010	-	5,5,5	1.41	0	5,5,5	4.15	4 (80%)
6	PGO	D	5008	-	4,4,4	0.76	0	4,4,4	0.65	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	-
3	PGR	B	5005	-	-	0/2/2/2	-
6	PGO	C	5007	-	-	0/2/2/2	-
5	GOL	C	5006	-	-	0/4/4/4	-
3	PGR	B	5004	-	-	0/2/2/2	-
3	PGR	A	5009	-	-	0/2/2/2	-
5	GOL	D	5010	-	-	3/4/4/4	-
6	PGO	D	5008	-	-	0/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5001	CO3	O1-C	4.57	1.41	1.25
4	C	5002	CO3	O1-C	4.03	1.39	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	5010	GOL	O3-C3-C2	7.24	142.98	110.38
5	D	5010	GOL	O2-C2-C1	4.26	126.81	109.18
5	D	5010	GOL	O1-C1-C2	3.03	124.01	110.38
5	D	5010	GOL	O2-C2-C3	2.44	119.28	109.18

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	5010	GOL	O1-C1-C2-C3
5	D	5010	GOL	O2-C2-C3-O3
5	D	5010	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	5010	GOL	3	0

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1/10 (10%)	1.15	0 100 100	21, 21, 21, 21	0
1	B	1/10 (10%)	0.03	0 100 100	17, 17, 17, 17	0
1	C	1/10 (10%)	0.37	0 100 100	18, 18, 18, 18	0
1	D	1/10 (10%)	-0.33	0 100 100	17, 17, 17, 17	0
All	All	4/40 (10%)	0.31	0 100 100	17, 17, 18, 21	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. 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	KPN	A	1005	22/23	0.93	0.12	16,22,26,28	0
1	KPN	B	2005	22/23	0.95	0.09	14,19,23,34	0
1	KPN	C	3005	22/23	0.96	0.09	11,14,19,20	0
1	KPN	D	4005	22/23	0.96	0.07	11,14,21,24	0
1	APN	C	3004	20/21	0.97	0.06	8,10,13,14	0
1	APN	D	4004	20/21	0.97	0.06	9,10,12,13	0
1	APN	A	1004	20/21	0.97	0.06	10,11,16,16	0
1	TPN	A	1006	19/20	0.97	0.07	10,13,22,22	0
1	TPN	B	2006	19/20	0.97	0.07	11,14,24,25	0
1	TPN	D	4006	19/20	0.97	0.07	9,10,13,13	0
1	GPN	C	3001	21/22	0.98	0.05	6,8,11,23	0
1	GPN	D	4001	21/22	0.98	0.05	6,8,11,16	0
1	GPN	D	4002	21/22	0.98	0.04	5,7,8,9	0
1	CPN	B	2003	18/19	0.98	0.04	6,8,11,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CPN	D	4003	18/19	0.98	0.05	6,7,10,14	0
1	GPN	A	1001	21/22	0.98	0.04	6,8,10,13	0
1	APN	B	2004	20/21	0.98	0.06	10,12,17,19	0
1	GPN	B	2001	21/22	0.98	0.04	6,7,9,9	0
1	GPN	A	1007	21/22	0.98	0.05	7,8,10,11	0
1	GPN	B	2007	21/22	0.98	0.04	6,8,12,13	0
1	GPN	D	4007	21/22	0.98	0.04	6,7,11,13	0
1	CPN	A	1008	18/19	0.98	0.04	5,6,7,8	0
1	CPN	A	1009	18/19	0.98	0.05	6,7,12,14	0
1	CPN	B	2009	18/19	0.98	0.06	7,8,13,14	0
1	CPN	A	1003	18/19	0.99	0.04	6,8,10,11	0
1	GPN	B	2002	21/22	0.99	0.04	5,7,8,9	0
1	GPN	C	3007	21/22	0.99	0.04	6,7,8,11	0
1	CPN	C	3003	18/19	0.99	0.05	7,7,9,10	0
1	GPN	C	3002	21/22	0.99	0.04	5,7,8,8	0
1	CPN	B	2008	18/19	0.99	0.04	5,6,8,8	0
1	CPN	C	3008	18/19	0.99	0.04	5,6,7,8	0
1	CPN	D	4008	18/19	0.99	0.04	5,6,7,8	0
1	TPN	C	3006	19/20	0.99	0.04	8,8,10,11	0
1	GPN	A	1002	21/22	0.99	0.04	6,6,8,8	0
1	CPN	C	3009	18/19	0.99	0.04	6,7,9,10	0
1	CPN	D	4009	18/19	0.99	0.04	6,7,9,10	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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($\text{\AA}^2$)	Q<0.9
5	GOL	D	5010	6/6	0.95	0.10	9,14,22,23	0
3	PGR	A	5009	5/5	0.97	0.09	8,14,16,24	0
3	PGR	B	5005	5/5	0.97	0.08	9,15,16,18	0
4	CO3	D	5001	4/4	0.97	0.08	11,11,14,16	0
2	EDO	A	5003	4/4	0.97	0.08	9,14,15,15	0
5	GOL	C	5006	6/6	0.98	0.07	8,15,20,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PGR	B	5004	5/5	0.98	0.07	10,13,14,15	0
6	PGO	C	5007	5/5	0.98	0.07	8,11,12,15	0
6	PGO	D	5008	5/5	0.98	0.05	8,10,10,13	0
4	CO3	C	5002	4/4	0.99	0.06	9,11,11,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.