



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:07 AM UTC

PDB ID : 9HBS / pdb_00009hbs
EMDB ID : EMD-52028
Title : TiLV-NP tetramer (pseudo-C2)
Authors : Arragain, B.; Cusack, S.
Deposited on : 2024-11-08
Resolution : 3.68 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

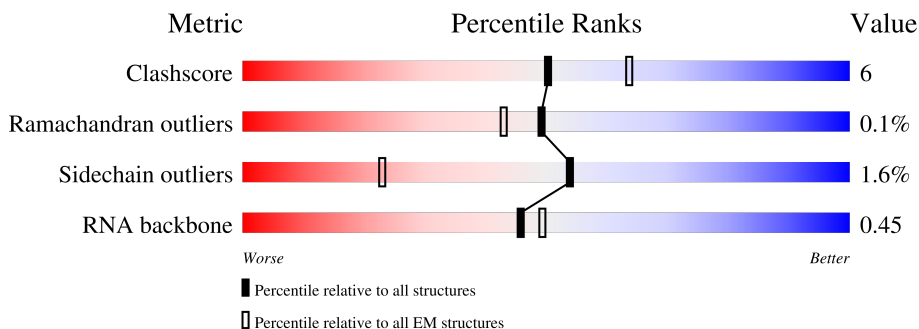
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.68 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	354	77% (green), 10% (yellow), 12% (grey)
1	B	354	79% (green), 10% (yellow), 11% (grey)
1	C	354	81% (green), 7% (yellow), 12% (grey)
1	D	354	78% (green), 10% (yellow), 12% (grey)
2	G	38	32% (yellow), 61% (orange), 8% (red)
2	H	38	29% (yellow), 50% (orange), 16% (red), 5% (grey)

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11044 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Tilapia Lake Virus nucleoprotein (segment 4).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	311	Total	C	N	O	S	0	0
			2387	1502	432	436	17		
1	B	316	Total	C	N	O	S	0	0
			2422	1521	438	446	17		
1	C	312	Total	C	N	O	S	0	0
			2391	1504	433	437	17		
1	D	313	Total	C	N	O	S	0	0
			2398	1506	435	440	17		

- Molecule 2 is a RNA chain called 40-mer vRNA loop.

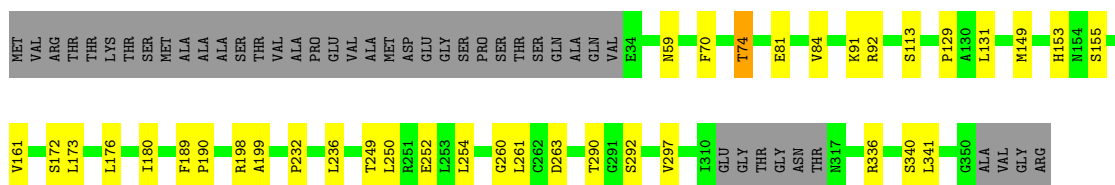
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	38	Total	C	N	O	P	0	0
			744	362	116	228	38		
2	H	36	Total	C	N	O	P	0	0
			702	342	108	216	36		

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. 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. 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.

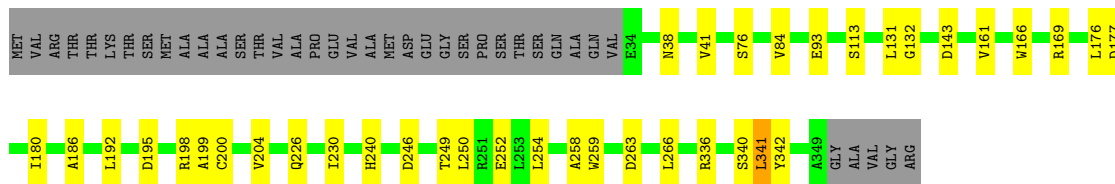
- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)

Chain A: 



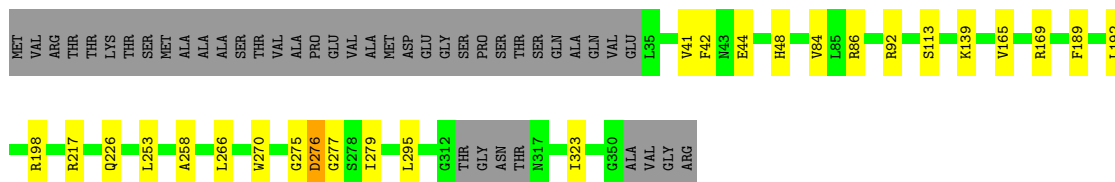
- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)

Chain B: 



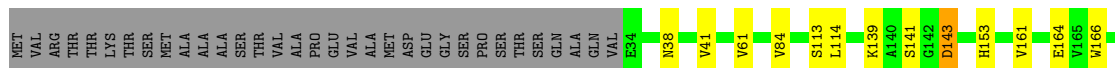
- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)

Chain C: 



- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)

Chain D: 





● Molecule 2: 40-mer vRNA loop



● Molecule 2: 40-mer vRNA loop



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	319609	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

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: P5P, Y5P

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	0.14	0/2428	0.27	0/3269
1	B	0.17	0/2464	0.29	0/3320
1	C	0.10	0/2432	0.25	0/3274
1	D	0.12	0/2439	0.26	0/3284
All	All	0.14	0/9763	0.27	0/13147

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	2387	0	2428	21	0
1	B	2422	0	2458	28	0
1	C	2391	0	2431	19	0
1	D	2398	0	2433	23	0
2	G	744	0	418	23	0
2	H	702	0	399	21	0
All	All	11044	0	10567	121	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 6.

All (121) 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:B:254:LEU:HD22	1:B:341:LEU:HD11	1.49	0.94
1:A:59:ASN:ND2	1:A:252:GLU:OE2	2.16	0.78
1:B:169:ARG:NH2	1:B:226:GLN:O	2.21	0.74
1:B:177:ASP:OD1	1:C:217:ARG:NH2	2.25	0.69
1:B:263:ASP:OD2	1:B:336:ARG:NE	2.26	0.69
1:B:226:GLN:OE1	1:B:259:TRP:NE1	2.26	0.68
1:A:129:PRO:HG3	1:A:149:MET:HE3	1.77	0.67
1:B:195:ASP:OD1	1:B:198:ARG:NH2	2.28	0.66
1:C:189:PHE:O	1:C:226:GLN:NE2	2.29	0.65
1:D:259:TRP:CD1	1:D:262:CYS:HG	2.14	0.65
1:C:275:GLY:O	1:C:277:GLY:N	2.31	0.64
1:C:198:ARG:NH1	2:H:5:P5P:O2'	2.31	0.63
1:B:169:ARG:NH1	1:B:230:ILE:HD12	2.14	0.62
1:D:263:ASP:OD2	1:D:336:ARG:NE	2.31	0.62
1:B:192:LEU:HD12	1:B:204:VAL:HG22	1.84	0.59
1:C:169:ARG:NH2	1:C:226:GLN:O	2.36	0.59
1:C:323:ILE:HG23	1:D:302:LEU:HD21	1.85	0.58
1:C:84:VAL:HG13	1:C:92:ARG:HG3	1.86	0.58
1:B:84:VAL:HG12	1:B:84:VAL:O	2.04	0.58
1:C:113:SER:O	1:C:113:SER:OG	2.17	0.58
1:A:290:THR:HG22	1:A:292:SER:H	1.70	0.57
1:A:263:ASP:OD2	1:A:336:ARG:NE	2.36	0.57
2:H:4:P5P:O2'	2:H:5:P5P:O5'	2.19	0.57
1:D:176:LEU:HD21	1:D:342:TYR:CD2	2.40	0.57
1:A:84:VAL:HG13	1:A:92:ARG:HG3	1.87	0.56
1:B:340:SER:OG	1:C:295:LEU:O	2.20	0.56
1:A:84:VAL:O	1:A:84:VAL:HG12	2.06	0.56
1:A:113:SER:O	1:A:113:SER:OG	2.18	0.55
2:H:27:P5P:H2'	2:H:28:Y5P:H6	1.89	0.55
1:C:84:VAL:HG12	1:C:84:VAL:O	2.07	0.54
1:B:249:THR:HG22	1:B:250:LEU:H	1.72	0.54
1:B:166:TRP:HB2	1:B:230:ILE:HG21	1.90	0.54
1:D:84:VAL:HG12	1:D:84:VAL:O	2.07	0.54
2:H:36:P5P:OP2	2:H:36:P5P:H8	2.08	0.54
1:C:44:GLU:O	1:C:48:HIS:ND1	2.40	0.54
1:A:131:LEU:HD11	2:G:7:Y5P:O4'	2.09	0.53
1:B:176:LEU:HD21	1:B:342:TYR:CD2	2.43	0.53
1:A:91:LYS:NZ	2:G:9:P5P:OP1	2.34	0.53
2:H:15:P5P:C6	2:H:16:Y5P:H4	2.39	0.53
2:G:15:P5P:C6	2:G:16:Y5P:H4	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:Y5P:H2'	2:H:29:P5P:H8	1.91	0.52
2:G:14:Y5P:H2'	2:G:15:P5P:H8	1.92	0.52
1:B:113:SER:O	1:B:113:SER:OG	2.23	0.52
2:H:29:P5P:H2'	2:H:30:P5P:H8	1.92	0.51
1:B:161:VAL:HG21	1:B:199:ALA:HB3	1.92	0.50
1:D:216:GLU:OE1	2:G:40:Y5P:H5	2.11	0.50
2:H:5:P5P:H8	2:H:5:P5P:OP2	2.12	0.50
1:B:249:THR:HG22	1:B:250:LEU:N	2.26	0.50
1:C:165:VAL:HG22	1:C:192:LEU:HD11	1.93	0.50
2:H:27:P5P:C6	2:H:28:Y5P:H4	2.41	0.50
2:G:27:P5P:C6	2:G:28:Y5P:H4	2.42	0.49
1:D:113:SER:O	1:D:113:SER:OG	2.25	0.49
1:D:258:ALA:CB	1:D:266:LEU:HD13	2.43	0.49
2:G:35:P5P:H8	2:G:35:P5P:O5'	2.12	0.49
2:H:26:Y5P:H2'	2:H:27:P5P:H8	1.93	0.49
2:G:26:Y5P:H2'	2:G:27:P5P:H8	1.94	0.49
1:C:277:GLY:O	1:C:279:ILE:HD12	2.12	0.49
1:A:297:VAL:HG21	1:D:259:TRP:HZ2	1.78	0.49
1:B:131:LEU:HD11	2:G:38:Y5P:O4'	2.13	0.48
1:B:240:HIS:NE2	1:B:246:ASP:OD2	2.46	0.48
2:H:16:Y5P:H2'	2:H:17:P5P:H8	1.95	0.48
2:G:29:P5P:H2'	2:G:30:P5P:H8	1.94	0.48
2:G:30:P5P:H2'	2:G:31:P5P:H8	1.96	0.48
1:A:297:VAL:HG21	1:D:259:TRP:CZ2	2.49	0.48
1:D:139:LYS:NZ	2:H:34:P5P:OP2	2.42	0.47
2:G:16:Y5P:H2'	2:G:17:P5P:H8	1.95	0.47
1:C:139:LYS:NZ	2:H:3:P5P:O3'	2.47	0.47
1:D:141:SER:OG	1:D:143:ASP:OD1	2.34	0.46
1:D:173:LEU:HD23	1:D:260:GLY:HA2	1.97	0.46
2:H:14:Y5P:H2'	2:H:15:P5P:H8	1.97	0.46
1:A:254:LEU:HD13	1:A:341:LEU:HD22	1.97	0.46
1:B:258:ALA:HB2	1:B:266:LEU:HD13	1.98	0.46
2:G:33:P5P:O2'	2:G:34:P5P:OP1	2.31	0.46
1:B:38:ASN:O	1:B:41:VAL:HG12	2.16	0.46
2:G:27:P5P:H2'	2:G:28:Y5P:H6	1.98	0.46
1:A:180:ILE:HG21	1:A:261:LEU:HD11	1.98	0.45
2:G:10:Y5P:H6	2:G:10:Y5P:O5'	2.16	0.45
1:D:166:TRP:HB2	1:D:230:ILE:HG21	1.99	0.45
2:G:28:Y5P:H2'	2:G:29:P5P:H8	1.97	0.45
1:A:173:LEU:HD23	1:A:260:GLY:HA2	1.98	0.44
1:D:254:LEU:HD22	1:D:341:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LEU:HD11	1:A:261:LEU:HD21	1.99	0.44
1:D:38:ASN:O	1:D:41:VAL:HG12	2.18	0.44
2:H:12:Y5P:H2'	2:H:13:Y5P:H6	1.99	0.44
1:D:61:VAL:HG13	1:D:114:LEU:HD21	1.99	0.44
1:D:161:VAL:HG21	1:D:199:ALA:HB3	1.98	0.44
1:B:258:ALA:CB	1:B:266:LEU:HD13	2.48	0.44
1:D:258:ALA:HB2	1:D:266:LEU:HD13	2.00	0.44
2:G:12:Y5P:H2'	2:G:13:Y5P:H6	2.00	0.44
2:G:17:P5P:C6	2:G:18:Y5P:H4	2.48	0.44
2:H:13:Y5P:H2'	2:H:14:Y5P:H6	1.99	0.44
1:B:131:LEU:HD12	1:B:132:GLY:N	2.34	0.43
1:D:321:GLU:HG3	1:D:322:CYS:H	1.82	0.43
1:B:93:GLU:OE2	1:C:86:ARG:NH1	2.51	0.43
1:C:258:ALA:HB2	1:C:266:LEU:HD13	2.01	0.43
1:D:143:ASP:OD1	1:D:143:ASP:N	2.50	0.43
1:B:254:LEU:HD22	1:B:341:LEU:CD1	2.35	0.43
2:H:39:Y5P:H6	2:H:39:Y5P:O5'	2.19	0.43
1:C:253:LEU:HD23	1:C:270:TRP:HB2	2.01	0.42
1:D:234:ARG:O	1:D:238:ILE:HD12	2.19	0.42
2:G:26:Y5P:H6	2:G:26:Y5P:O5'	2.19	0.42
2:G:36:P5P:OP2	2:G:36:P5P:H8	2.19	0.42
2:H:30:P5P:H2'	2:H:31:P5P:H8	2.02	0.42
1:B:161:VAL:HG11	1:B:200:CYS:HB2	2.00	0.42
1:A:176:LEU:CD1	1:A:261:LEU:HD21	2.50	0.42
2:H:15:P5P:H2'	2:H:16:Y5P:H6	2.01	0.41
2:H:35:P5P:H8	2:H:35:P5P:O5'	2.20	0.41
1:C:84:VAL:CG1	1:C:92:ARG:HE	2.33	0.41
2:G:17:P5P:H2'	2:G:18:Y5P:H6	2.02	0.41
1:D:169:ARG:NH2	1:D:226:GLN:O	2.54	0.41
2:G:13:Y5P:H2'	2:G:14:Y5P:H6	2.02	0.41
1:A:161:VAL:HG21	1:A:199:ALA:HB3	2.03	0.41
1:A:249:THR:HG22	1:A:250:LEU:N	2.36	0.41
1:A:232:PRO:O	1:A:236:LEU:N	2.52	0.41
1:B:132:GLY:HA3	2:G:38:Y5P:H5	2.03	0.41
1:A:70:PHE:O	1:A:74:THR:OG1	2.21	0.40
1:B:143:ASP:OD1	1:B:143:ASP:N	2.54	0.40
1:A:189:PHE:CG	1:A:190:PRO:HA	2.57	0.40
1:B:180:ILE:CG2	1:B:186:ALA:HB2	2.51	0.40
1:C:41:VAL:HG13	1:C:42:PHE:N	2.37	0.40
2:H:33:P5P:O2'	2:H:34:P5P:OP1	2.32	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/354 (87%)	301 (98%)	6 (2%)	0	100	100
1	B	314/354 (89%)	301 (96%)	13 (4%)	0	100	100
1	C	308/354 (87%)	294 (96%)	13 (4%)	1 (0%)	36	65
1	D	309/354 (87%)	298 (96%)	11 (4%)	0	100	100
All	All	1238/1416 (87%)	1194 (96%)	43 (4%)	1 (0%)	49	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	276	ASP

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	A	253/285 (89%)	246 (97%)	7 (3%)	38	58
1	B	257/285 (90%)	254 (99%)	3 (1%)	63	71
1	C	253/285 (89%)	252 (100%)	1 (0%)	84	81
1	D	254/285 (89%)	249 (98%)	5 (2%)	48	64
All	All	1017/1140 (89%)	1001 (98%)	16 (2%)	54	67

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	THR
1	A	81	GLU
1	A	153	HIS
1	A	155	SER
1	A	172	SER
1	A	198	ARG
1	A	340	SER
1	B	76	SER
1	B	252	GLU
1	B	341	LEU
1	C	276	ASP
1	D	143	ASP
1	D	153	HIS
1	D	164	GLU
1	D	288	GLN
1	D	341	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	226	GLN
1	B	148	GLN
1	B	315	ASN
1	D	181	GLN
1	D	240	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	36/38 (94%)	7 (19%)	0
2	H	33/38 (86%)	11 (33%)	0
All	All	69/76 (90%)	18 (26%)	0

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	6	Y5P
2	G	11	Y5P
2	G	30	P5P
2	G	34	P5P

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Mol	Chain	Res	Type
2	G	36	P5P
2	G	37	Y5P
2	G	41	P5P
2	H	4	P5P
2	H	5	P5P
2	H	6	Y5P
2	H	7	Y5P
2	H	30	P5P
2	H	34	P5P
2	H	36	P5P
2	H	37	Y5P
2	H	38	Y5P
2	H	39	Y5P
2	H	40	Y5P

There are no RNA pucker outliers to report.

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

74 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
2	P5P	G	15	2	20,23,24	0.46	0	27,33,36	0.72	1 (3%)
2	Y5P	H	14	2	14,19,20	4.54	2 (14%)	18,26,29	1.39	2 (11%)
2	P5P	H	34	2	20,23,24	0.46	0	27,33,36	0.75	1 (3%)
2	Y5P	G	10	2	14,19,20	4.23	2 (14%)	18,26,29	1.01	1 (5%)
2	Y5P	G	28	2	14,19,20	4.23	2 (14%)	18,26,29	1.01	1 (5%)
2	P5P	G	24	2	20,23,24	0.97	2 (10%)	27,33,36	1.85	3 (11%)
2	P5P	H	32	2	20,23,24	0.46	0	27,33,36	0.71	1 (3%)
2	P5P	H	4	2	20,23,24	0.45	0	27,33,36	0.68	1 (3%)
2	Y5P	H	19	2	14,19,20	4.53	2 (14%)	18,26,29	1.36	2 (11%)
2	Y5P	G	11	2	14,19,20	4.14	2 (14%)	18,26,29	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	Y5P	H	18	2	14,19,20	4.20	2 (14%)	18,26,29	1.01	1 (5%)
2	Y5P	H	7	2	14,19,20	4.19	2 (14%)	18,26,29	1.01	1 (5%)
2	P5P	H	25	2	20,23,24	0.45	0	27,33,36	0.70	1 (3%)
2	P5P	G	1	2	20,23,24	0.46	0	27,33,36	0.70	1 (3%)
2	Y5P	G	16	2	14,19,20	4.59	2 (14%)	18,26,29	1.38	2 (11%)
2	Y5P	G	20	2	14,19,20	4.56	2 (14%)	18,26,29	1.35	2 (11%)
2	P5P	G	29	2	20,23,24	0.96	2 (10%)	27,33,36	1.86	3 (11%)
2	Y5P	G	26	2	14,19,20	4.59	2 (14%)	18,26,29	1.39	2 (11%)
2	P5P	G	31	2	20,23,24	0.97	2 (10%)	27,33,36	1.85	3 (11%)
2	P5P	G	35	2	20,23,24	0.45	0	27,33,36	0.74	1 (3%)
2	Y5P	H	38	2	14,19,20	4.20	2 (14%)	18,26,29	1.02	1 (5%)
2	Y5P	G	39	2	14,19,20	4.20	2 (14%)	18,26,29	1.03	1 (5%)
2	Y5P	H	37	2	14,19,20	4.20	2 (14%)	18,26,29	1.01	1 (5%)
2	Y5P	H	6	2	14,19,20	4.17	2 (14%)	18,26,29	1.04	1 (5%)
2	Y5P	H	12	2	14,19,20	4.57	2 (14%)	18,26,29	1.39	2 (11%)
2	Y5P	G	8	2	14,19,20	4.22	2 (14%)	18,26,29	1.04	1 (5%)
2	P5P	G	4	2	20,23,24	0.45	0	27,33,36	0.73	1 (3%)
2	Y5P	H	11	2	14,19,20	4.16	2 (14%)	18,26,29	1.04	1 (5%)
2	Y5P	H	40	2	14,19,20	4.57	2 (14%)	18,26,29	1.35	2 (11%)
2	Y5P	H	39	2	14,19,20	4.19	2 (14%)	18,26,29	1.04	1 (5%)
2	Y5P	G	14	2	14,19,20	4.53	2 (14%)	18,26,29	1.39	2 (11%)
2	P5P	H	5	2	20,23,24	0.45	0	27,33,36	0.70	1 (3%)
2	Y5P	H	20	2	14,19,20	4.57	2 (14%)	18,26,29	1.35	2 (11%)
2	P5P	G	36	2	20,23,24	0.45	0	27,33,36	0.73	1 (3%)
2	P5P	H	1	2	20,23,24	0.45	0	27,33,36	0.69	1 (3%)
2	Y5P	G	37	2	14,19,20	4.18	2 (14%)	18,26,29	1.01	1 (5%)
2	P5P	G	9	2	20,23,24	0.45	0	27,33,36	0.72	1 (3%)
2	Y5P	G	18	2	14,19,20	4.24	2 (14%)	18,26,29	1.01	1 (5%)
2	P5P	G	2	2	20,23,24	0.47	0	27,33,36	0.70	1 (3%)
2	Y5P	H	28	2	14,19,20	4.27	2 (14%)	18,26,29	1.01	1 (5%)
2	P5P	G	30	2	20,23,24	0.44	0	27,33,36	0.74	1 (3%)
2	P5P	H	3	2	20,23,24	0.46	0	27,33,36	0.70	1 (3%)
2	Y5P	H	16	2	14,19,20	4.61	2 (14%)	18,26,29	1.35	2 (11%)
2	P5P	G	5	2	20,23,24	0.46	0	27,33,36	0.69	1 (3%)
2	P5P	G	17	2	20,23,24	0.96	2 (10%)	27,33,36	1.82	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	Y5P	G	6	2	14,19,20	4.22	2 (14%)	18,26,29	1.03	1 (5%)
2	Y5P	H	26	2	14,19,20	4.58	2 (14%)	18,26,29	1.36	2 (11%)
2	Y5P	G	12	2	14,19,20	4.57	2 (14%)	18,26,29	1.38	2 (11%)
2	P5P	H	35	2	20,23,24	0.45	0	27,33,36	0.71	1 (3%)
2	P5P	H	33	2	20,23,24	0.45	0	27,33,36	0.73	1 (3%)
2	P5P	H	15	2	20,23,24	0.45	0	27,33,36	0.72	1 (3%)
2	Y5P	H	8	2	14,19,20	4.19	2 (14%)	18,26,29	1.02	1 (5%)
2	Y5P	H	13	2	14,19,20	4.17	2 (14%)	18,26,29	1.04	1 (5%)
2	P5P	H	36	2	20,23,24	0.45	0	27,33,36	0.72	1 (3%)
2	Y5P	G	40	2	14,19,20	4.58	2 (14%)	18,26,29	1.33	2 (11%)
2	P5P	G	34	2	20,23,24	0.46	0	27,33,36	0.77	1 (3%)
2	P5P	H	17	2	20,23,24	0.97	2 (10%)	27,33,36	1.84	3 (11%)
2	P5P	G	41	2	20,23,24	0.96	3 (15%)	27,33,36	1.85	3 (11%)
2	P5P	H	29	2	20,23,24	0.96	2 (10%)	27,33,36	1.88	3 (11%)
2	Y5P	H	10	2	14,19,20	4.09	2 (14%)	18,26,29	1.04	1 (5%)
2	P5P	G	33	2	20,23,24	0.45	0	27,33,36	0.72	1 (3%)
2	Y5P	G	19	2	14,19,20	4.54	2 (14%)	18,26,29	1.35	2 (11%)
2	P5P	H	30	2	20,23,24	0.44	0	27,33,36	0.75	1 (3%)
2	P5P	H	2	2	20,23,24	0.45	0	27,33,36	0.70	1 (3%)
2	P5P	G	3	2	20,23,24	0.45	0	27,33,36	0.69	1 (3%)
2	P5P	G	25	2	20,23,24	0.46	0	27,33,36	0.68	1 (3%)
2	P5P	H	24	2	20,23,24	0.97	2 (10%)	27,33,36	1.85	3 (11%)
2	P5P	G	27	2	20,23,24	0.95	2 (10%)	27,33,36	1.88	4 (14%)
2	P5P	H	31	2	20,23,24	0.98	2 (10%)	27,33,36	1.83	3 (11%)
2	P5P	G	32	2	20,23,24	0.44	0	27,33,36	0.74	1 (3%)
2	Y5P	G	7	2	14,19,20	4.18	2 (14%)	18,26,29	1.02	1 (5%)
2	P5P	H	27	2	20,23,24	0.96	2 (10%)	27,33,36	1.86	4 (14%)
2	Y5P	G	13	2	14,19,20	4.13	2 (14%)	18,26,29	1.04	1 (5%)
2	Y5P	G	38	2	14,19,20	4.22	2 (14%)	18,26,29	1.01	1 (5%)

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	P5P	G	15	2	-	0/7/25/26	0/3/3/3
2	Y5P	H	14	2	-	1/7/33/34	0/2/2/2
2	P5P	H	34	2	-	3/7/25/26	0/3/3/3
2	Y5P	G	10	2	-	1/7/33/34	0/2/2/2
2	Y5P	G	28	2	-	1/7/33/34	0/2/2/2
2	P5P	G	24	2	-	0/7/25/26	0/3/3/3
2	P5P	H	32	2	-	2/7/25/26	0/3/3/3
2	P5P	H	4	2	-	1/7/25/26	0/3/3/3
2	Y5P	H	19	2	-	1/7/33/34	0/2/2/2
2	Y5P	G	11	2	-	3/7/33/34	0/2/2/2
2	Y5P	H	18	2	-	1/7/33/34	0/2/2/2
2	Y5P	H	7	2	-	1/7/33/34	0/2/2/2
2	P5P	H	25	2	-	0/7/25/26	0/3/3/3
2	P5P	G	1	2	-	0/7/25/26	0/3/3/3
2	Y5P	G	16	2	-	1/7/33/34	0/2/2/2
2	Y5P	G	20	2	-	1/7/33/34	0/2/2/2
2	P5P	G	29	2	-	0/7/25/26	0/3/3/3
2	Y5P	G	26	2	-	1/7/33/34	0/2/2/2
2	P5P	G	31	2	-	0/7/25/26	0/3/3/3
2	P5P	G	35	2	-	0/7/25/26	0/3/3/3
2	Y5P	H	38	2	-	3/7/33/34	0/2/2/2
2	Y5P	G	39	2	-	3/7/33/34	0/2/2/2
2	Y5P	H	37	2	-	2/7/33/34	0/2/2/2
2	Y5P	H	6	2	-	2/7/33/34	0/2/2/2
2	Y5P	H	12	2	-	1/7/33/34	0/2/2/2
2	Y5P	G	8	2	-	1/7/33/34	0/2/2/2
2	P5P	G	4	2	-	0/7/25/26	0/3/3/3
2	Y5P	H	11	2	-	1/7/33/34	0/2/2/2
2	Y5P	H	40	2	-	3/7/33/34	0/2/2/2
2	Y5P	H	39	2	-	3/7/33/34	0/2/2/2
2	Y5P	G	14	2	-	1/7/33/34	0/2/2/2
2	P5P	H	5	2	-	2/7/25/26	0/3/3/3
2	Y5P	H	20	2	-	1/7/33/34	0/2/2/2
2	P5P	G	36	2	-	2/7/25/26	0/3/3/3
2	P5P	H	1	2	-	0/7/25/26	0/3/3/3
2	Y5P	G	37	2	-	2/7/33/34	0/2/2/2
2	P5P	G	9	2	-	0/7/25/26	0/3/3/3
2	Y5P	G	18	2	-	1/7/33/34	0/2/2/2
2	P5P	G	2	2	-	0/7/25/26	0/3/3/3
2	Y5P	H	28	2	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P5P	G	30	2	-	2/7/25/26	0/3/3/3
2	P5P	H	3	2	-	0/7/25/26	0/3/3/3
2	Y5P	H	16	2	-	1/7/33/34	0/2/2/2
2	P5P	G	5	2	-	0/7/25/26	0/3/3/3
2	P5P	G	17	2	-	0/7/25/26	0/3/3/3
2	Y5P	G	6	2	-	3/7/33/34	0/2/2/2
2	Y5P	H	26	2	-	1/7/33/34	0/2/2/2
2	Y5P	G	12	2	-	1/7/33/34	0/2/2/2
2	P5P	H	35	2	-	0/7/25/26	0/3/3/3
2	P5P	H	33	2	-	0/7/25/26	0/3/3/3
2	P5P	H	15	2	-	0/7/25/26	0/3/3/3
2	Y5P	H	8	2	-	1/7/33/34	0/2/2/2
2	Y5P	H	13	2	-	1/7/33/34	0/2/2/2
2	P5P	H	36	2	-	2/7/25/26	0/3/3/3
2	Y5P	G	40	2	-	3/7/33/34	0/2/2/2
2	P5P	G	34	2	-	3/7/25/26	0/3/3/3
2	P5P	H	17	2	-	0/7/25/26	0/3/3/3
2	P5P	G	41	2	-	1/7/25/26	0/3/3/3
2	P5P	H	29	2	-	0/7/25/26	0/3/3/3
2	Y5P	H	10	2	-	1/7/33/34	0/2/2/2
2	P5P	G	33	2	-	0/7/25/26	0/3/3/3
2	Y5P	G	19	2	-	1/7/33/34	0/2/2/2
2	P5P	H	30	2	-	2/7/25/26	0/3/3/3
2	P5P	H	2	2	-	2/7/25/26	0/3/3/3
2	P5P	G	3	2	-	1/7/25/26	0/3/3/3
2	P5P	G	25	2	-	0/7/25/26	0/3/3/3
2	P5P	H	24	2	-	0/7/25/26	0/3/3/3
2	P5P	G	27	2	-	0/7/25/26	0/3/3/3
2	P5P	H	31	2	-	0/7/25/26	0/3/3/3
2	P5P	G	32	2	-	2/7/25/26	0/3/3/3
2	Y5P	G	7	2	-	1/7/33/34	0/2/2/2
2	P5P	H	27	2	-	0/7/25/26	0/3/3/3
2	Y5P	G	13	2	-	1/7/33/34	0/2/2/2
2	Y5P	G	38	2	-	1/7/33/34	0/2/2/2

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	18	Y5P	C2-N3	13.57	1.37	1.27
2	H	28	Y5P	C2-N3	13.56	1.37	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	18	Y5P	C2-N3	13.51	1.37	1.27
2	G	28	Y5P	C2-N3	13.37	1.37	1.27
2	G	16	Y5P	C4-N3	-13.37	1.33	1.46
2	G	8	Y5P	C2-N3	13.36	1.37	1.27
2	H	40	Y5P	C4-N3	-13.35	1.33	1.46
2	G	6	Y5P	C2-N3	13.33	1.37	1.27
2	G	40	Y5P	C4-N3	-13.32	1.33	1.46
2	H	16	Y5P	C4-N3	-13.30	1.33	1.46
2	G	10	Y5P	C2-N3	13.30	1.37	1.27
2	H	20	Y5P	C4-N3	-13.29	1.33	1.46
2	H	38	Y5P	C2-N3	13.27	1.37	1.27
2	G	12	Y5P	C4-N3	-13.25	1.33	1.46
2	G	39	Y5P	C2-N3	13.25	1.37	1.27
2	H	12	Y5P	C4-N3	-13.24	1.33	1.46
2	H	39	Y5P	C2-N3	13.23	1.37	1.27
2	H	7	Y5P	C2-N3	13.22	1.37	1.27
2	G	14	Y5P	C4-N3	-13.22	1.33	1.46
2	G	26	Y5P	C4-N3	-13.20	1.33	1.46
2	H	8	Y5P	C2-N3	13.19	1.37	1.27
2	G	38	Y5P	C2-N3	13.19	1.37	1.27
2	G	19	Y5P	C4-N3	-13.18	1.33	1.46
2	G	11	Y5P	C2-N3	13.18	1.37	1.27
2	G	7	Y5P	C2-N3	13.16	1.37	1.27
2	H	13	Y5P	C2-N3	13.16	1.37	1.27
2	H	14	Y5P	C4-N3	-13.16	1.33	1.46
2	H	26	Y5P	C4-N3	-13.13	1.33	1.46
2	H	6	Y5P	C2-N3	13.12	1.37	1.27
2	H	37	Y5P	C2-N3	13.12	1.37	1.27
2	G	20	Y5P	C4-N3	-13.11	1.33	1.46
2	G	13	Y5P	C2-N3	13.11	1.37	1.27
2	H	11	Y5P	C2-N3	13.10	1.37	1.27
2	G	37	Y5P	C2-N3	13.03	1.37	1.27
2	H	19	Y5P	C4-N3	-13.02	1.34	1.46
2	H	10	Y5P	C2-N3	12.69	1.37	1.27
2	H	26	Y5P	C2-N3	10.94	1.35	1.27
2	H	16	Y5P	C2-N3	10.90	1.35	1.27
2	G	26	Y5P	C2-N3	10.90	1.35	1.27
2	G	20	Y5P	C2-N3	10.86	1.35	1.27
2	H	19	Y5P	C2-N3	10.81	1.35	1.27
2	G	40	Y5P	C2-N3	10.75	1.35	1.27
2	G	12	Y5P	C2-N3	10.75	1.35	1.27
2	H	12	Y5P	C2-N3	10.73	1.35	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	16	Y5P	C2-N3	10.72	1.35	1.27
2	H	20	Y5P	C2-N3	10.70	1.35	1.27
2	H	14	Y5P	C2-N3	10.70	1.35	1.27
2	G	19	Y5P	C2-N3	10.65	1.35	1.27
2	H	40	Y5P	C2-N3	10.65	1.35	1.27
2	G	14	Y5P	C2-N3	10.55	1.35	1.27
2	G	38	Y5P	C4-N3	-8.61	1.38	1.46
2	G	37	Y5P	C4-N3	-8.59	1.38	1.46
2	H	37	Y5P	C4-N3	-8.56	1.38	1.46
2	G	10	Y5P	C4-N3	-8.50	1.38	1.46
2	H	10	Y5P	C4-N3	-8.44	1.38	1.46
2	G	39	Y5P	C4-N3	-8.41	1.38	1.46
2	H	8	Y5P	C4-N3	-8.41	1.38	1.46
2	H	39	Y5P	C4-N3	-8.39	1.38	1.46
2	G	7	Y5P	C4-N3	-8.39	1.38	1.46
2	G	6	Y5P	C4-N3	-8.39	1.38	1.46
2	H	7	Y5P	C4-N3	-8.39	1.38	1.46
2	G	28	Y5P	C4-N3	-8.37	1.38	1.46
2	G	8	Y5P	C4-N3	-8.36	1.38	1.46
2	H	38	Y5P	C4-N3	-8.34	1.38	1.46
2	H	6	Y5P	C4-N3	-8.34	1.38	1.46
2	H	11	Y5P	C4-N3	-8.33	1.38	1.46
2	H	28	Y5P	C4-N3	-8.32	1.38	1.46
2	H	13	Y5P	C4-N3	-8.32	1.38	1.46
2	G	18	Y5P	C4-N3	-8.16	1.38	1.46
2	G	13	Y5P	C4-N3	-8.12	1.38	1.46
2	G	11	Y5P	C4-N3	-8.06	1.38	1.46
2	H	18	Y5P	C4-N3	-7.95	1.38	1.46
2	H	17	P5P	C6-N1	2.55	1.39	1.34
2	G	24	P5P	C6-N1	2.54	1.39	1.34
2	H	31	P5P	C6-N1	2.54	1.39	1.34
2	G	17	P5P	C6-N1	2.51	1.39	1.34
2	H	27	P5P	C6-N1	2.51	1.39	1.34
2	H	24	P5P	C6-N1	2.51	1.39	1.34
2	G	27	P5P	C6-N1	2.50	1.39	1.34
2	G	29	P5P	C6-N1	2.48	1.39	1.34
2	G	31	P5P	C6-N1	2.48	1.39	1.34
2	H	29	P5P	C6-N1	2.43	1.39	1.34
2	G	41	P5P	C6-N1	2.36	1.39	1.34
2	H	24	P5P	C2-N1	2.25	1.37	1.33
2	G	24	P5P	C2-N1	2.24	1.37	1.33
2	H	29	P5P	C2-N1	2.22	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	27	P5P	C2-N1	2.20	1.37	1.33
2	H	27	P5P	C2-N1	2.19	1.37	1.33
2	H	31	P5P	C2-N1	2.18	1.37	1.33
2	G	29	P5P	C2-N1	2.18	1.37	1.33
2	H	17	P5P	C2-N1	2.18	1.37	1.33
2	G	31	P5P	C2-N1	2.17	1.37	1.33
2	G	41	P5P	C2-N1	2.16	1.37	1.33
2	G	17	P5P	C2-N1	2.15	1.37	1.33
2	G	41	P5P	C6-C5	2.05	1.42	1.39

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	41	P5P	C6-N1-C2	7.80	125.01	115.80
2	G	27	P5P	C6-N1-C2	7.77	124.97	115.80
2	H	29	P5P	C6-N1-C2	7.73	124.92	115.80
2	H	27	P5P	C6-N1-C2	7.72	124.91	115.80
2	G	24	P5P	C6-N1-C2	7.70	124.89	115.80
2	G	29	P5P	C6-N1-C2	7.70	124.89	115.80
2	H	24	P5P	C6-N1-C2	7.69	124.87	115.80
2	G	31	P5P	C6-N1-C2	7.62	124.79	115.80
2	H	17	P5P	C6-N1-C2	7.61	124.78	115.80
2	H	31	P5P	C6-N1-C2	7.60	124.77	115.80
2	G	17	P5P	C6-N1-C2	7.54	124.70	115.80
2	H	14	Y5P	C5-C4-N3	4.93	122.10	114.15
2	G	14	Y5P	C5-C4-N3	4.93	122.09	114.15
2	H	12	Y5P	C5-C4-N3	4.92	122.09	114.15
2	G	26	Y5P	C5-C4-N3	4.90	122.05	114.15
2	G	12	Y5P	C5-C4-N3	4.88	122.02	114.15
2	G	16	Y5P	C5-C4-N3	4.87	122.00	114.15
2	H	19	Y5P	C5-C4-N3	4.86	121.98	114.15
2	G	19	Y5P	C5-C4-N3	4.85	121.96	114.15
2	H	26	Y5P	C5-C4-N3	4.83	121.94	114.15
2	G	20	Y5P	C5-C4-N3	4.80	121.89	114.15
2	H	40	Y5P	C5-C4-N3	4.79	121.88	114.15
2	H	20	Y5P	C5-C4-N3	4.79	121.87	114.15
2	H	16	Y5P	C5-C4-N3	4.76	121.82	114.15
2	G	40	Y5P	C5-C4-N3	4.74	121.79	114.15
2	H	29	P5P	C5-C6-N1	-4.17	111.50	121.90
2	G	29	P5P	C5-C6-N1	-4.16	111.54	121.90
2	G	41	P5P	C5-C6-N1	-4.14	111.60	121.90
2	G	31	P5P	C5-C6-N1	-4.13	111.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	24	P5P	C5-C6-N1	-4.12	111.64	121.90
2	G	27	P5P	C5-C6-N1	-4.11	111.65	121.90
2	H	31	P5P	C5-C6-N1	-4.10	111.68	121.90
2	H	24	P5P	C5-C6-N1	-4.10	111.68	121.90
2	G	17	P5P	C5-C6-N1	-4.08	111.73	121.90
2	H	17	P5P	C5-C6-N1	-4.08	111.74	121.90
2	H	27	P5P	C5-C6-N1	-4.07	111.77	121.90
2	G	8	Y5P	N1-C2-N3	-3.85	114.71	125.39
2	G	6	Y5P	N1-C2-N3	-3.83	114.76	125.39
2	H	6	Y5P	N1-C2-N3	-3.83	114.76	125.39
2	H	39	Y5P	N1-C2-N3	-3.83	114.76	125.39
2	G	39	Y5P	N1-C2-N3	-3.81	114.82	125.39
2	H	8	Y5P	N1-C2-N3	-3.79	114.88	125.39
2	G	38	Y5P	N1-C2-N3	-3.78	114.91	125.39
2	H	38	Y5P	N1-C2-N3	-3.78	114.91	125.39
2	G	37	Y5P	N1-C2-N3	-3.77	114.93	125.39
2	G	10	Y5P	N1-C2-N3	-3.77	114.94	125.39
2	H	7	Y5P	N1-C2-N3	-3.76	114.97	125.39
2	G	18	Y5P	N1-C2-N3	-3.76	114.97	125.39
2	H	13	Y5P	N1-C2-N3	-3.75	114.99	125.39
2	G	7	Y5P	N1-C2-N3	-3.75	114.99	125.39
2	G	13	Y5P	N1-C2-N3	-3.75	115.00	125.39
2	H	28	Y5P	N1-C2-N3	-3.74	115.01	125.39
2	H	18	Y5P	N1-C2-N3	-3.74	115.02	125.39
2	H	11	Y5P	N1-C2-N3	-3.74	115.03	125.39
2	G	28	Y5P	N1-C2-N3	-3.73	115.04	125.39
2	H	10	Y5P	N1-C2-N3	-3.73	115.05	125.39
2	H	37	Y5P	N1-C2-N3	-3.73	115.05	125.39
2	G	11	Y5P	N1-C2-N3	-3.72	115.07	125.39
2	H	29	P5P	C6-C5-C4	2.84	119.35	116.24
2	G	31	P5P	C6-C5-C4	2.81	119.32	116.24
2	G	29	P5P	C6-C5-C4	2.73	119.22	116.24
2	H	17	P5P	C6-C5-C4	2.61	119.09	116.24
2	G	33	P5P	C6-N1-C2	2.58	118.85	115.80
2	G	27	P5P	C6-C5-C4	2.57	119.05	116.24
2	G	17	P5P	C6-C5-C4	2.56	119.04	116.24
2	H	24	P5P	C6-C5-C4	2.53	119.00	116.24
2	G	24	P5P	C6-C5-C4	2.52	118.99	116.24
2	H	27	P5P	C6-C5-C4	2.51	118.99	116.24
2	H	31	P5P	C6-C5-C4	2.49	118.97	116.24
2	G	36	P5P	C6-N1-C2	2.49	118.73	115.80
2	G	4	P5P	C6-N1-C2	2.48	118.73	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	33	P5P	C6-N1-C2	2.48	118.73	115.80
2	G	9	P5P	C6-N1-C2	2.46	118.70	115.80
2	H	30	P5P	C6-N1-C2	2.46	118.70	115.80
2	G	41	P5P	C6-C5-C4	2.43	118.90	116.24
2	G	35	P5P	C6-N1-C2	2.42	118.66	115.80
2	G	1	P5P	C6-N1-C2	2.41	118.64	115.80
2	H	2	P5P	C6-N1-C2	2.41	118.64	115.80
2	H	35	P5P	C6-N1-C2	2.40	118.64	115.80
2	G	30	P5P	C6-N1-C2	2.40	118.64	115.80
2	H	5	P5P	C6-N1-C2	2.40	118.64	115.80
2	G	5	P5P	C6-N1-C2	2.37	118.60	115.80
2	H	4	P5P	C6-N1-C2	2.36	118.58	115.80
2	H	36	P5P	C6-N1-C2	2.35	118.58	115.80
2	G	3	P5P	C6-N1-C2	2.35	118.58	115.80
2	G	15	P5P	C6-N1-C2	2.35	118.57	115.80
2	H	32	P5P	C6-N1-C2	2.34	118.57	115.80
2	G	2	P5P	C6-N1-C2	2.33	118.55	115.80
2	H	15	P5P	C6-N1-C2	2.33	118.55	115.80
2	H	3	P5P	C6-N1-C2	2.32	118.54	115.80
2	H	1	P5P	C6-N1-C2	2.30	118.52	115.80
2	H	34	P5P	C6-N1-C2	2.28	118.49	115.80
2	G	16	Y5P	N1-C2-N3	-2.26	119.13	125.39
2	G	26	Y5P	N1-C2-N3	-2.24	119.17	125.39
2	H	19	Y5P	N1-C2-N3	-2.22	119.23	125.39
2	G	34	P5P	C6-N1-C2	2.22	118.42	115.80
2	H	16	Y5P	N1-C2-N3	-2.21	119.25	125.39
2	G	12	Y5P	N1-C2-N3	-2.21	119.25	125.39
2	G	32	P5P	C6-N1-C2	2.21	118.41	115.80
2	G	20	Y5P	N1-C2-N3	-2.21	119.27	125.39
2	H	26	Y5P	N1-C2-N3	-2.19	119.31	125.39
2	H	40	Y5P	N1-C2-N3	-2.19	119.32	125.39
2	H	20	Y5P	N1-C2-N3	-2.19	119.32	125.39
2	H	14	Y5P	N1-C2-N3	-2.19	119.33	125.39
2	G	19	Y5P	N1-C2-N3	-2.18	119.34	125.39
2	G	40	Y5P	N1-C2-N3	-2.17	119.36	125.39
2	H	12	Y5P	N1-C2-N3	-2.14	119.45	125.39
2	H	25	P5P	C6-N1-C2	2.13	118.32	115.80
2	G	14	Y5P	N1-C2-N3	-2.12	119.50	125.39
2	G	25	P5P	C6-N1-C2	2.11	118.29	115.80
2	G	27	P5P	N1-C2-N3	-2.03	123.87	127.33
2	H	27	P5P	N1-C2-N3	-2.01	123.91	127.33

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	5	P5P	C3'-C4'-C5'-O5'
2	H	5	P5P	O4'-C4'-C5'-O5'
2	G	6	Y5P	O4'-C1'-N1-C2
2	H	6	Y5P	O4'-C1'-N1-C2
2	G	10	Y5P	O4'-C1'-N1-C2
2	G	18	Y5P	O4'-C1'-N1-C2
2	G	19	Y5P	O4'-C1'-N1-C2
2	H	19	Y5P	O4'-C1'-N1-C2
2	G	20	Y5P	O4'-C1'-N1-C2
2	H	20	Y5P	O4'-C1'-N1-C2
2	G	26	Y5P	O4'-C1'-N1-C2
2	H	26	Y5P	O4'-C1'-N1-C2
2	G	36	P5P	O4'-C4'-C5'-O5'
2	H	36	P5P	O4'-C4'-C5'-O5'
2	G	37	Y5P	C4'-C5'-O5'-P
2	H	37	Y5P	C4'-C5'-O5'-P
2	H	37	Y5P	O4'-C1'-N1-C2
2	H	10	Y5P	O4'-C1'-N1-C2
2	G	11	Y5P	O4'-C1'-N1-C2
2	H	11	Y5P	O4'-C1'-N1-C2
2	G	12	Y5P	O4'-C1'-N1-C2
2	H	12	Y5P	O4'-C1'-N1-C2
2	G	13	Y5P	O4'-C1'-N1-C2
2	H	13	Y5P	O4'-C1'-N1-C2
2	G	14	Y5P	O4'-C1'-N1-C2
2	H	14	Y5P	O4'-C1'-N1-C2
2	G	16	Y5P	O4'-C1'-N1-C2
2	H	16	Y5P	O4'-C1'-N1-C2
2	H	18	Y5P	O4'-C1'-N1-C2
2	G	28	Y5P	O4'-C1'-N1-C2
2	H	28	Y5P	O4'-C1'-N1-C2
2	G	37	Y5P	O4'-C1'-N1-C2
2	G	39	Y5P	O4'-C1'-N1-C2
2	H	39	Y5P	O4'-C1'-N1-C2
2	G	11	Y5P	O4'-C4'-C5'-O5'
2	G	30	P5P	C3'-C4'-C5'-O5'
2	G	30	P5P	O4'-C4'-C5'-O5'
2	G	36	P5P	C3'-C4'-C5'-O5'
2	H	36	P5P	C3'-C4'-C5'-O5'
2	H	8	Y5P	O4'-C1'-N1-C2
2	H	30	P5P	C3'-C4'-C5'-O5'
2	H	30	P5P	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	H	39	Y5P	O4'-C4'-C5'-O5'
2	G	40	Y5P	C3'-C4'-C5'-O5'
2	H	6	Y5P	C4'-C5'-O5'-P
2	G	8	Y5P	O4'-C1'-N1-C2
2	G	6	Y5P	C3'-C4'-C5'-O5'
2	G	11	Y5P	C3'-C4'-C5'-O5'
2	G	32	P5P	C3'-C4'-C5'-O5'
2	G	34	P5P	C3'-C4'-C5'-O5'
2	H	40	Y5P	C3'-C4'-C5'-O5'
2	G	38	Y5P	O4'-C1'-N1-C2
2	H	38	Y5P	O4'-C1'-N1-C2
2	G	6	Y5P	O4'-C4'-C5'-O5'
2	G	34	P5P	O4'-C4'-C5'-O5'
2	H	34	P5P	C3'-C4'-C5'-O5'
2	G	40	Y5P	O4'-C4'-C5'-O5'
2	H	2	P5P	C3'-C4'-C5'-O5'
2	H	39	Y5P	C3'-C4'-C5'-O5'
2	H	7	Y5P	O4'-C1'-N1-C2
2	G	32	P5P	O4'-C4'-C5'-O5'
2	H	32	P5P	C3'-C4'-C5'-O5'
2	G	40	Y5P	O4'-C1'-N1-C2
2	H	40	Y5P	O4'-C1'-N1-C2
2	G	39	Y5P	O4'-C4'-C5'-O5'
2	G	7	Y5P	O4'-C1'-N1-C6
2	H	2	P5P	O4'-C4'-C5'-O5'
2	H	34	P5P	O4'-C4'-C5'-O5'
2	H	40	Y5P	O4'-C4'-C5'-O5'
2	H	32	P5P	O4'-C4'-C5'-O5'
2	H	4	P5P	C4'-C5'-O5'-P
2	H	38	Y5P	O4'-C4'-C5'-O5'
2	G	34	P5P	C2'-C1'-N9-C8
2	G	41	P5P	O4'-C4'-C5'-O5'
2	H	34	P5P	C2'-C1'-N9-C8
2	G	3	P5P	C3'-C4'-C5'-O5'
2	G	39	Y5P	C3'-C4'-C5'-O5'
2	H	38	Y5P	C4'-C5'-O5'-P

There are no ring outliers.

42 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	15	P5P	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	14	Y5P	2	0
2	H	34	P5P	2	0
2	G	10	Y5P	1	0
2	G	28	Y5P	3	0
2	H	4	P5P	1	0
2	G	16	Y5P	2	0
2	G	29	P5P	2	0
2	G	26	Y5P	2	0
2	G	31	P5P	1	0
2	G	35	P5P	1	0
2	H	12	Y5P	1	0
2	H	39	Y5P	1	0
2	G	14	Y5P	2	0
2	H	5	P5P	3	0
2	G	36	P5P	1	0
2	G	9	P5P	1	0
2	G	18	Y5P	2	0
2	H	28	Y5P	3	0
2	G	30	P5P	2	0
2	H	3	P5P	1	0
2	H	16	Y5P	3	0
2	G	17	P5P	3	0
2	H	26	Y5P	1	0
2	G	12	Y5P	1	0
2	H	35	P5P	1	0
2	H	33	P5P	1	0
2	H	15	P5P	3	0
2	H	13	Y5P	2	0
2	H	36	P5P	1	0
2	G	40	Y5P	1	0
2	G	34	P5P	1	0
2	H	17	P5P	1	0
2	H	29	P5P	2	0
2	G	33	P5P	1	0
2	H	30	P5P	2	0
2	G	27	P5P	3	0
2	H	31	P5P	1	0
2	G	7	Y5P	1	0
2	H	27	P5P	3	0
2	G	13	Y5P	2	0
2	G	38	Y5P	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	1
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	20:Y5P	O3'	24:P5P	P	15.60
1	H	20:Y5P	O3'	24:P5P	P	15.58

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52028. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.