



Full wwPDB EM Validation Report ⓘ

Mar 3, 2025 – 12:50 pm GMT

PDB ID : 9HBT
EMDB ID : EMD-52029
Title : TiLV-NP pentamer (pseudo-C5)
Authors : Arragain, B.; Cusack, S.
Deposited on : 2024-11-08
Resolution : 3.46 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 : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

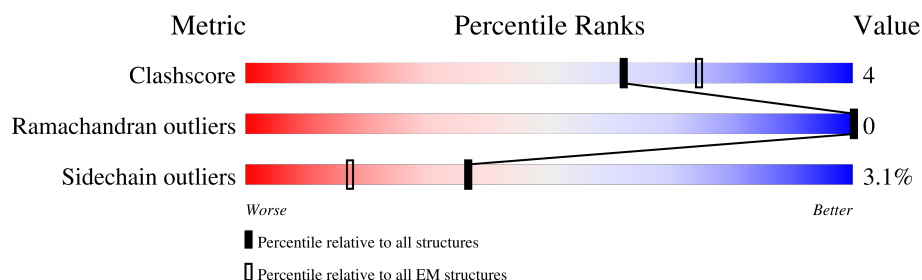
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.46 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	79% 10% • 10%
1	B	354	81% 8% 10%
1	C	354	79% 9% • 11%
1	D	354	80% 9% • 10%
1	E	354	79% 9% • 11%
2	O	52	• 13% 8% 77%
2	P	52	6% 13% • 77%
2	Q	52	10% 8% 6% 77%
2	R	52	6% 10% 8% 77%

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Mol	Chain	Length	Quality of chain
2	S	52	<div><div><div></div><div></div><div></div></div><div>10%10%•77%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13327 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	317	Total	C	N	O	S	1	0
			2433	1527	443	446	17		
1	B	317	Total	C	N	O	S	1	0
			2433	1527	443	446	17		
1	C	314	Total	C	N	O	S	1	0
			2414	1517	439	441	17		
1	D	317	Total	C	N	O	S	1	0
			2433	1527	443	446	17		
1	E	316	Total	C	N	O	S	1	0
			2429	1525	442	445	17		


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

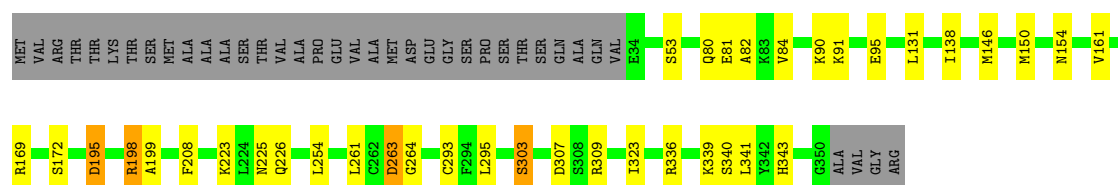
Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	12	Total	C	N	O	P	0	0
			237	115	38	72	12		
2	P	12	Total	C	N	O	P	0	0
			237	115	38	72	12		
2	Q	12	Total	C	N	O	P	0	0
			237	115	38	72	12		
2	R	12	Total	C	N	O	P	0	0
			237	115	38	72	12		
2	S	12	Total	C	N	O	P	0	0
			237	115	38	72	12		

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.

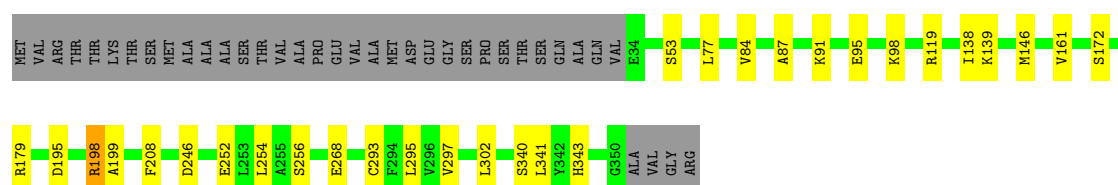
- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)

Chain A: 




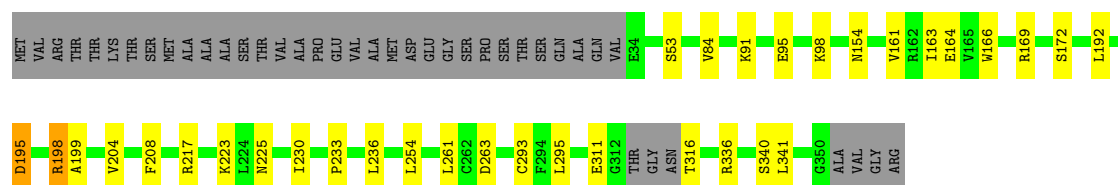
- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)

Chain B: 




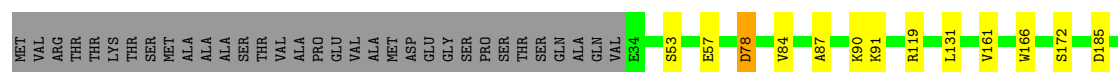
- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)

Chain C: 

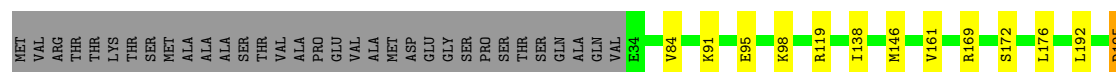
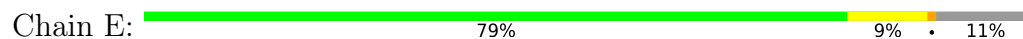


- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)

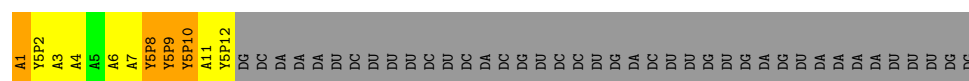
Chain D: 



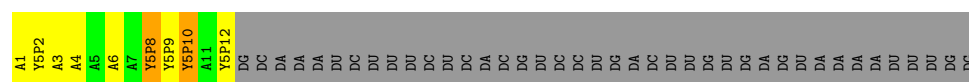
- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)



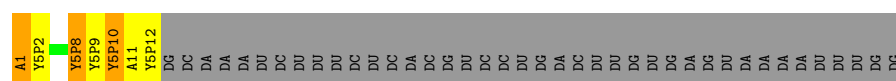
- Molecule 2: 40-mer vRNA loop



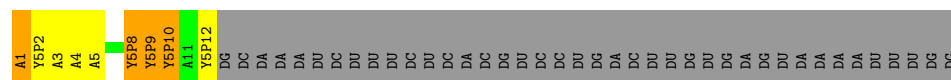
- Molecule 2: 40-mer vRNA loop



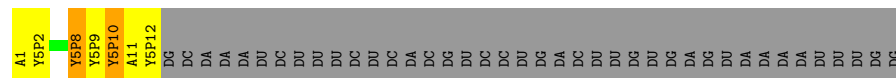
- Molecule 2: 40-mer vRNA loop



- 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, C1	Depositor
Number of particles used	352053	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 ($e^-/\text{\AA}^2$)	40	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	0.25	0/2475	0.48	0/3334
1	B	0.24	0/2475	0.47	0/3334
1	C	0.24	0/2455	0.48	0/3305
1	D	0.25	0/2475	0.48	0/3334
1	E	0.24	0/2471	0.48	0/3329
All	All	0.24	0/12351	0.48	0/16636

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	2433	0	2469	30	0
1	B	2433	0	2469	21	0
1	C	2414	0	2452	24	0
1	D	2433	0	2469	21	0
1	E	2429	0	2466	26	0
2	O	237	0	131	11	0
2	P	237	0	131	5	0
2	Q	237	0	131	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	237	0	131	7	0
2	S	237	0	131	4	0
All	All	13327	0	12980	108	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 4.

All (108) 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:295:LEU:O	1:E:340:SER:OG	1.93	0.87
1:B:340:SER:OG	1:C:295:LEU:O	1.94	0.84
1:A:340:SER:OG	1:B:295:LEU:O	1.96	0.83
1:C:340:SER:OG	1:D:295:LEU:O	1.97	0.81
1:D:340:SER:OG	1:E:295:LEU:O	1.99	0.80
1:D:338:GLY:O	1:E:308:SER:OG	2.01	0.78
1:A:225:ASN:ND2	2:O:1:P5P:OP2	2.19	0.75
1:E:95:GLU:OE1	1:E:98:LYS:NZ	2.24	0.70
1:D:225:ASN:ND2	2:R:1:P5P:OP2	2.24	0.69
1:D:254:LEU:HD13	1:D:341:LEU:HD22	1.72	0.69
1:C:225:ASN:ND2	2:Q:1:P5P:OP2	2.27	0.67
1:C:95:GLU:OE1	1:C:98:LYS:NZ	2.27	0.67
1:A:261:LEU:O	1:B:297:VAL:HG22	1.95	0.66
1:C:198[B]:ARG:NH2	2:Q:8:Y5P:O2'	2.27	0.66
1:D:261:LEU:O	1:E:297:VAL:HG22	1.95	0.66
1:D:208:PHE:CD1	2:R:10:Y5P:H4A	2.30	0.66
1:B:343:HIS:NE2	1:C:293:CYS:O	2.28	0.65
1:E:91:LYS:NZ	2:S:11:P5P:OP1	2.30	0.64
1:A:293:CYS:O	1:E:343:HIS:NE2	2.31	0.62
1:D:323:ILE:HG23	1:E:302:LEU:HD21	1.82	0.62
1:A:254:LEU:HD13	1:A:341:LEU:HD22	1.82	0.61
1:E:198[B]:ARG:NH2	2:S:8:Y5P:O2'	2.34	0.61
1:A:323:ILE:HG23	1:B:302:LEU:HD21	1.82	0.61
1:D:318:LEU:HD12	1:E:311:GLU:OE2	2.01	0.60
1:E:169:ARG:NH2	1:E:226:GLN:O	2.33	0.60
1:E:84:VAL:O	1:E:84:VAL:HG12	2.03	0.59
1:B:84:VAL:HG12	1:B:84:VAL:O	2.03	0.59
1:A:208:PHE:CD1	2:O:10:Y5P:H4A	2.39	0.58
1:B:179:ARG:NH1	1:C:217:ARG:O	2.35	0.58
1:A:84:VAL:O	1:A:84:VAL:HG12	2.04	0.58
1:E:321:GLU:N	1:E:321:GLU:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:PHE:CD1	2:S:10:Y5P:H4A	2.41	0.56
1:C:208:PHE:CD1	2:Q:10:Y5P:H4A	2.40	0.56
1:A:154:ASN:OD1	2:O:8:Y5P:N3	2.38	0.56
1:C:84:VAL:HG12	1:C:84:VAL:O	2.05	0.56
1:C:254:LEU:HD13	1:C:341:LEU:HD22	1.88	0.56
1:E:254:LEU:HD13	1:E:341:LEU:HD22	1.88	0.56
1:D:198[B]:ARG:NH2	2:R:8:Y5P:O2'	2.39	0.55
1:B:208:PHE:CD1	2:P:10:Y5P:H4A	2.42	0.54
1:D:84:VAL:HG12	1:D:84:VAL:O	2.07	0.54
1:A:91:LYS:NZ	2:O:11:P5P:OP1	2.41	0.54
1:A:138:ILE:HD12	1:A:146:MET:HG2	1.90	0.54
1:A:307:ASP:OD1	1:A:309:ARG:N	2.42	0.53
1:C:254:LEU:HD22	1:C:341:LEU:HD11	1.90	0.53
1:B:77:LEU:O	1:B:98:LYS:NZ	2.33	0.52
1:B:139:LYS:NZ	2:P:6:P5P:OP2	2.38	0.52
1:B:268:GLU:N	1:B:268:GLU:OE1	2.42	0.52
2:O:6:P5P:H3'	2:O:7:P5P:H8	1.91	0.52
1:E:161:VAL:HG21	1:E:199:ALA:HB3	1.92	0.51
1:C:261:LEU:O	1:D:297:VAL:HG22	2.10	0.51
1:A:80:GLN:OE1	1:A:81:GLU:OE1	2.28	0.51
1:A:169:ARG:NH2	1:A:226:GLN:O	2.44	0.51
1:B:161:VAL:HG21	1:B:199:ALA:HB3	1.93	0.51
1:A:131:LEU:HD11	2:O:9:Y5P:O4'	2.12	0.49
1:A:254:LEU:HD22	1:A:341:LEU:HD11	1.93	0.49
1:A:198[B]:ARG:HH11	2:O:10:Y5P:H5	1.77	0.49
1:C:263:ASP:OD2	1:C:336:ARG:NH2	2.42	0.49
1:B:252:GLU:O	1:B:256:SER:OG	2.28	0.48
1:A:150:MET:CE	2:O:8:Y5P:H4A	2.43	0.48
1:A:263:ASP:OD2	1:A:336:ARG:NH2	2.44	0.47
1:C:198[B]:ARG:HH11	2:Q:10:Y5P:H5	1.78	0.47
1:E:138:ILE:HD12	1:E:146:MET:HG2	1.94	0.47
2:O:3:P5P:H2'	2:O:4:P5P:O4'	2.14	0.47
1:D:161:VAL:HG21	1:D:199:ALA:HB3	1.96	0.47
1:A:161:VAL:HG21	1:A:199:ALA:HB3	1.97	0.46
1:D:234:ARG:O	1:D:238:ILE:HD12	2.15	0.46
1:C:169:ARG:NH1	1:C:230:ILE:HD12	2.31	0.46
1:E:195:ASP:N	1:E:195:ASP:OD1	2.48	0.46
1:E:317:ASN:N	1:E:317:ASN:OD1	2.49	0.46
1:D:185:ASP:O	1:D:191:TYR:OH	2.28	0.46
1:A:150:MET:HE2	2:O:8:Y5P:H4A	1.98	0.45
1:A:323:ILE:CG2	1:B:302:LEU:HD21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:HIS:NE2	1:B:293:CYS:O	2.45	0.45
1:C:192:LEU:HD12	1:C:204:VAL:HG22	1.99	0.45
1:A:138:ILE:HD12	1:A:146:MET:CG	2.47	0.45
1:D:198[B]:ARG:HH11	2:R:10:Y5P:H5	1.82	0.45
1:A:303:SER:HB3	1:E:318:LEU:HD22	1.97	0.44
2:R:3:P5P:H2'	2:R:4:P5P:O4'	2.17	0.44
1:E:176:LEU:HD11	1:E:342:TYR:CE2	2.53	0.44
1:B:138:ILE:HD12	1:B:146:MET:HG2	1.99	0.43
1:C:161:VAL:HG21	1:C:199:ALA:HB3	1.99	0.43
1:A:264:GLY:N	1:A:339:LYS:O	2.51	0.43
1:B:87:ALA:HB1	1:B:91:LYS:CG	2.48	0.43
1:A:195:ASP:OD1	1:A:195:ASP:N	2.52	0.43
1:D:131:LEU:HD11	2:R:9:Y5P:O4'	2.18	0.43
1:E:198[B]:ARG:HH11	2:S:10:Y5P:H5	1.84	0.43
1:C:91:LYS:NZ	2:Q:11:P5P:OP1	2.51	0.43
1:D:78:ASP:N	1:D:78:ASP:OD1	2.52	0.43
1:D:87:ALA:HB1	1:D:91:LYS:CG	2.50	0.42
1:C:163:ILE:HG13	1:C:236:LEU:HD23	2.00	0.42
1:E:84:VAL:O	1:E:84:VAL:CG1	2.68	0.42
1:A:198[B]:ARG:NH2	2:O:8:Y5P:O2'	2.40	0.41
1:A:82:ALA:HB1	1:A:95:GLU:HB3	2.03	0.41
1:B:198[B]:ARG:NH2	2:P:8:Y5P:O2'	2.54	0.41
1:C:84:VAL:O	1:C:84:VAL:CG1	2.68	0.41
1:D:166:TRP:HB2	1:D:230:ILE:HG21	2.02	0.41
1:C:154:ASN:OD1	2:Q:8:Y5P:N3	2.54	0.41
1:C:164:GLU:HG2	1:C:192:LEU:HD13	2.02	0.41
1:B:84:VAL:O	1:B:84:VAL:CG1	2.68	0.41
2:P:3:P5P:H2'	2:P:4:P5P:O4'	2.21	0.41
1:C:166:TRP:CD2	1:C:233:PRO:HD3	2.56	0.41
1:B:254:LEU:HD13	1:B:341:LEU:HD22	2.02	0.41
1:E:238:ILE:HG22	1:E:238:ILE:O	2.21	0.41
1:C:195:ASP:OD1	1:C:195:ASP:N	2.54	0.40
2:R:4:P5P:H2'	2:R:5:P5P:H8	2.02	0.40
1:E:192:LEU:HD12	1:E:204:VAL:HG22	2.04	0.40
1:B:198[B]:ARG:HH11	2:P:10:Y5P:H5	1.86	0.40
1:D:259:TRP:CZ2	1:E:297:VAL:HG21	2.57	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	316/354 (89%)	307 (97%)	9 (3%)	0	100	100
1	B	316/354 (89%)	311 (98%)	5 (2%)	0	100	100
1	C	311/354 (88%)	308 (99%)	3 (1%)	0	100	100
1	D	316/354 (89%)	310 (98%)	6 (2%)	0	100	100
1	E	315/354 (89%)	311 (99%)	4 (1%)	0	100	100
All	All	1574/1770 (89%)	1547 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	257/285 (90%)	248 (96%)	9 (4%)	31	61
1	B	257/285 (90%)	249 (97%)	8 (3%)	35	64
1	C	255/285 (90%)	247 (97%)	8 (3%)	35	64
1	D	257/285 (90%)	247 (96%)	10 (4%)	27	58
1	E	257/285 (90%)	248 (96%)	9 (4%)	31	61
All	All	1283/1425 (90%)	1239 (97%)	44 (3%)	37	61

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	90	LYS
1	A	172	SER
1	A	195	ASP
1	A	198[A]	ARG
1	A	198[B]	ARG
1	A	223	LYS
1	A	263	ASP
1	A	303	SER
1	B	53	SER
1	B	95	GLU
1	B	119	ARG
1	B	172	SER
1	B	195	ASP
1	B	198[A]	ARG
1	B	198[B]	ARG
1	B	246	ASP
1	C	53	SER
1	C	172	SER
1	C	195	ASP
1	C	198[A]	ARG
1	C	198[B]	ARG
1	C	223	LYS
1	C	311	GLU
1	C	316	THR
1	D	53	SER
1	D	57	GLU
1	D	78	ASP
1	D	90	LYS
1	D	119	ARG
1	D	172	SER
1	D	195	ASP
1	D	198[A]	ARG
1	D	198[B]	ARG
1	D	262	CYS
1	E	119	ARG
1	E	172	SER
1	E	195	ASP
1	E	198[A]	ARG
1	E	198[B]	ARG
1	E	246	ASP
1	E	288	GLN
1	E	303	SER

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Mol	Chain	Res	Type
1	E	308	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	B	240	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

60 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	Y5P	S	12	2	14,19,20	2.31	1 (7%)	18,26,29	0.99	1 (5%)
2	Y5P	Q	12	2	14,19,20	2.32	1 (7%)	18,26,29	1.00	1 (5%)
2	P5P	O	4	2	16,23,24	0.79	0	14,33,36	0.75	0
2	Y5P	S	2	2	14,19,20	3.70	1 (7%)	18,26,29	0.78	1 (5%)
2	P5P	R	1	2	16,23,24	1.33	3 (18%)	14,33,36	1.95	2 (14%)
2	P5P	Q	6	2	16,23,24	0.77	0	14,33,36	0.78	0
2	P5P	Q	4	2	16,23,24	0.79	0	14,33,36	0.74	0
2	P5P	S	3	2	16,23,24	0.78	0	14,33,36	0.73	0
2	P5P	Q	3	2	16,23,24	0.79	0	14,33,36	0.72	0
2	Y5P	O	12	2	14,19,20	2.35	1 (7%)	18,26,29	0.99	1 (5%)
2	P5P	R	3	2	16,23,24	0.79	0	14,33,36	0.73	0
2	P5P	P	1	2	16,23,24	1.33	3 (18%)	14,33,36	1.95	2 (14%)
2	Y5P	O	8	2	14,19,20	2.36	1 (7%)	18,26,29	0.99	1 (5%)
2	P5P	Q	11	2	16,23,24	0.78	0	14,33,36	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	Y5P	R	2	2	14,19,20	3.66	1 (7%)	18,26,29	0.79	1 (5%)
2	Y5P	Q	10	2	14,19,20	2.34	1 (7%)	18,26,29	0.99	1 (5%)
2	P5P	P	11	2	16,23,24	0.77	0	14,33,36	0.73	0
2	P5P	P	3	2	16,23,24	0.77	0	14,33,36	0.73	0
2	Y5P	O	2	2	14,19,20	3.69	1 (7%)	18,26,29	0.79	1 (5%)
2	P5P	S	1	2	16,23,24	1.32	3 (18%)	14,33,36	1.93	2 (14%)
2	Y5P	P	2	2	14,19,20	3.66	1 (7%)	18,26,29	0.78	1 (5%)
2	P5P	S	11	2	16,23,24	0.79	0	14,33,36	0.73	0
2	P5P	S	4	2	16,23,24	0.79	0	14,33,36	0.73	0
2	P5P	Q	7	2	16,23,24	0.78	0	14,33,36	0.73	0
2	Y5P	R	10	2	14,19,20	2.36	1 (7%)	18,26,29	0.99	1 (5%)
2	Y5P	O	9	2	14,19,20	2.37	1 (7%)	18,26,29	0.99	1 (5%)
2	Y5P	Q	9	2	14,19,20	2.35	1 (7%)	18,26,29	1.00	1 (5%)
2	P5P	R	6	2	16,23,24	0.78	0	14,33,36	0.75	0
2	P5P	O	5	2	16,23,24	0.78	0	14,33,36	0.75	0
2	P5P	O	1	2	16,23,24	1.31	2 (12%)	14,33,36	1.96	2 (14%)
2	P5P	O	3	2	16,23,24	0.81	0	14,33,36	0.74	0
2	P5P	R	7	2	16,23,24	0.78	0	14,33,36	0.72	0
2	P5P	S	6	2	16,23,24	0.77	0	14,33,36	0.78	0
2	P5P	S	7	2	16,23,24	0.79	0	14,33,36	0.73	0
2	Y5P	P	8	2	14,19,20	2.35	1 (7%)	18,26,29	0.99	1 (5%)
2	P5P	Q	1	2	16,23,24	1.33	3 (18%)	14,33,36	1.92	2 (14%)
2	Y5P	R	9	2	14,19,20	2.34	1 (7%)	18,26,29	0.99	1 (5%)
2	Y5P	P	12	2	14,19,20	2.34	1 (7%)	18,26,29	1.00	1 (5%)
2	P5P	P	6	2	16,23,24	0.78	0	14,33,36	0.74	0
2	P5P	R	5	2	16,23,24	0.77	0	14,33,36	0.76	0
2	P5P	Q	5	2	16,23,24	0.77	0	14,33,36	0.75	0
2	P5P	S	5	2	16,23,24	0.77	0	14,33,36	0.74	0
2	P5P	P	7	2	16,23,24	0.78	0	14,33,36	0.73	0
2	Y5P	P	10	2	14,19,20	2.35	1 (7%)	18,26,29	1.00	1 (5%)
2	P5P	O	11	2	16,23,24	0.76	0	14,33,36	0.74	0
2	Y5P	R	12	2	14,19,20	2.34	1 (7%)	18,26,29	0.99	1 (5%)
2	Y5P	Q	2	2	14,19,20	3.68	1 (7%)	18,26,29	0.78	1 (5%)
2	Y5P	P	9	2	14,19,20	2.35	1 (7%)	18,26,29	1.00	1 (5%)
2	Y5P	O	10	2	14,19,20	2.37	1 (7%)	18,26,29	0.99	1 (5%)
2	P5P	R	4	2	16,23,24	0.78	0	14,33,36	0.75	0
2	Y5P	S	8	2	14,19,20	2.36	1 (7%)	18,26,29	1.00	1 (5%)
2	P5P	R	11	2	16,23,24	0.79	0	14,33,36	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P5P	O	6	2	16,23,24	0.79	0	14,33,36	0.77	0
2	Y5P	S	10	2	14,19,20	2.35	1 (7%)	18,26,29	0.99	1 (5%)
2	P5P	O	7	2	16,23,24	0.79	0	14,33,36	0.77	0
2	P5P	P	4	2	16,23,24	0.79	0	14,33,36	0.73	0
2	Y5P	S	9	2	14,19,20	2.35	1 (7%)	18,26,29	0.99	1 (5%)
2	Y5P	R	8	2	14,19,20	2.34	1 (7%)	18,26,29	1.01	1 (5%)
2	P5P	P	5	2	16,23,24	0.78	0	14,33,36	0.73	0
2	Y5P	Q	8	2	14,19,20	2.36	1 (7%)	18,26,29	1.00	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	Y5P	S	12	2	-	1/7/33/34	0/2/2/2
2	Y5P	Q	12	2	-	1/7/33/34	0/2/2/2
2	P5P	O	4	2	-	0/3/25/26	0/3/3/3
2	Y5P	S	2	2	-	4/7/33/34	0/2/2/2
2	P5P	R	1	2	-	2/3/25/26	0/3/3/3
2	P5P	Q	6	2	-	3/3/25/26	0/3/3/3
2	P5P	Q	4	2	-	0/3/25/26	0/3/3/3
2	P5P	S	3	2	-	2/3/25/26	0/3/3/3
2	P5P	Q	3	2	-	3/3/25/26	0/3/3/3
2	Y5P	O	12	2	-	1/7/33/34	0/2/2/2
2	P5P	R	3	2	-	3/3/25/26	0/3/3/3
2	P5P	P	1	2	-	2/3/25/26	0/3/3/3
2	Y5P	O	8	2	-	1/7/33/34	0/2/2/2
2	P5P	Q	11	2	-	0/3/25/26	0/3/3/3
2	Y5P	R	2	2	-	4/7/33/34	0/2/2/2
2	Y5P	Q	10	2	-	2/7/33/34	0/2/2/2
2	P5P	P	11	2	-	0/3/25/26	0/3/3/3
2	P5P	P	3	2	-	2/3/25/26	0/3/3/3
2	Y5P	O	2	2	-	4/7/33/34	0/2/2/2
2	P5P	S	1	2	-	2/3/25/26	0/3/3/3
2	Y5P	P	2	2	-	4/7/33/34	0/2/2/2
2	P5P	S	11	2	-	0/3/25/26	0/3/3/3
2	P5P	S	4	2	-	0/3/25/26	0/3/3/3
2	P5P	Q	7	2	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y5P	R	10	2	-	2/7/33/34	0/2/2/2
2	Y5P	O	9	2	-	2/7/33/34	0/2/2/2
2	Y5P	Q	9	2	-	1/7/33/34	0/2/2/2
2	P5P	R	6	2	-	0/3/25/26	0/3/3/3
2	P5P	O	5	2	-	0/3/25/26	0/3/3/3
2	P5P	O	1	2	-	2/3/25/26	0/3/3/3
2	P5P	O	3	2	-	2/3/25/26	0/3/3/3
2	P5P	R	7	2	-	0/3/25/26	0/3/3/3
2	P5P	S	6	2	-	1/3/25/26	0/3/3/3
2	P5P	S	7	2	-	0/3/25/26	0/3/3/3
2	Y5P	P	8	2	-	1/7/33/34	0/2/2/2
2	P5P	Q	1	2	-	2/3/25/26	0/3/3/3
2	Y5P	R	9	2	-	1/7/33/34	0/2/2/2
2	Y5P	P	12	2	-	1/7/33/34	0/2/2/2
2	P5P	P	6	2	-	0/3/25/26	0/3/3/3
2	P5P	R	5	2	-	0/3/25/26	0/3/3/3
2	P5P	Q	5	2	-	0/3/25/26	0/3/3/3
2	P5P	S	5	2	-	0/3/25/26	0/3/3/3
2	P5P	P	7	2	-	0/3/25/26	0/3/3/3
2	Y5P	P	10	2	-	2/7/33/34	0/2/2/2
2	P5P	O	11	2	-	0/3/25/26	0/3/3/3
2	Y5P	R	12	2	-	1/7/33/34	0/2/2/2
2	Y5P	Q	2	2	-	3/7/33/34	0/2/2/2
2	Y5P	P	9	2	-	1/7/33/34	0/2/2/2
2	Y5P	O	10	2	-	2/7/33/34	0/2/2/2
2	P5P	R	4	2	-	0/3/25/26	0/3/3/3
2	Y5P	S	8	2	-	4/7/33/34	0/2/2/2
2	P5P	R	11	2	-	0/3/25/26	0/3/3/3
2	P5P	O	6	2	-	1/3/25/26	0/3/3/3
2	Y5P	S	10	2	-	2/7/33/34	0/2/2/2
2	P5P	O	7	2	-	0/3/25/26	0/3/3/3
2	P5P	P	4	2	-	0/3/25/26	0/3/3/3
2	Y5P	S	9	2	-	1/7/33/34	0/2/2/2
2	Y5P	R	8	2	-	3/7/33/34	0/2/2/2
2	P5P	P	5	2	-	0/3/25/26	0/3/3/3
2	Y5P	Q	8	2	-	4/7/33/34	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	2	Y5P	C4-N3	-13.68	1.33	1.46
2	O	2	Y5P	C4-N3	-13.65	1.33	1.46
2	Q	2	Y5P	C4-N3	-13.60	1.33	1.46
2	P	2	Y5P	C4-N3	-13.55	1.33	1.46
2	R	2	Y5P	C4-N3	-13.55	1.33	1.46
2	O	9	Y5P	C4-N3	-8.74	1.38	1.46
2	O	10	Y5P	C4-N3	-8.71	1.38	1.46
2	Q	8	Y5P	C4-N3	-8.69	1.38	1.46
2	O	8	Y5P	C4-N3	-8.69	1.38	1.46
2	S	8	Y5P	C4-N3	-8.67	1.38	1.46
2	Q	9	Y5P	C4-N3	-8.67	1.38	1.46
2	R	10	Y5P	C4-N3	-8.66	1.38	1.46
2	P	9	Y5P	C4-N3	-8.66	1.38	1.46
2	S	9	Y5P	C4-N3	-8.66	1.38	1.46
2	O	12	Y5P	C4-N3	-8.64	1.38	1.46
2	S	10	Y5P	C4-N3	-8.62	1.38	1.46
2	P	10	Y5P	C4-N3	-8.62	1.38	1.46
2	P	8	Y5P	C4-N3	-8.62	1.38	1.46
2	R	9	Y5P	C4-N3	-8.62	1.38	1.46
2	R	12	Y5P	C4-N3	-8.60	1.38	1.46
2	P	12	Y5P	C4-N3	-8.59	1.38	1.46
2	R	8	Y5P	C4-N3	-8.58	1.38	1.46
2	Q	10	Y5P	C4-N3	-8.58	1.38	1.46
2	Q	12	Y5P	C4-N3	-8.53	1.38	1.46
2	S	12	Y5P	C4-N3	-8.50	1.38	1.46
2	R	1	P5P	C6-N1	4.07	1.39	1.32
2	Q	1	P5P	C6-N1	4.06	1.39	1.32
2	O	1	P5P	C6-N1	4.03	1.39	1.32
2	P	1	P5P	C6-N1	4.02	1.39	1.32
2	S	1	P5P	C6-N1	4.02	1.39	1.32
2	P	1	P5P	C8-N7	-2.17	1.30	1.34
2	P	1	P5P	C2-N1	2.15	1.37	1.33
2	Q	1	P5P	C8-N7	-2.13	1.30	1.34
2	Q	1	P5P	C2-N1	2.13	1.37	1.33
2	O	1	P5P	C2-N1	2.12	1.37	1.33
2	R	1	P5P	C2-N1	2.11	1.37	1.33
2	S	1	P5P	C2-N1	2.08	1.37	1.33
2	S	1	P5P	C8-N7	-2.08	1.31	1.34
2	R	1	P5P	C8-N7	-2.07	1.31	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	P5P	C6-N1-C2	6.46	125.09	115.84
2	P	1	P5P	C6-N1-C2	6.45	125.07	115.84
2	R	1	P5P	C6-N1-C2	6.44	125.06	115.84
2	S	1	P5P	C6-N1-C2	6.39	124.99	115.84
2	Q	1	P5P	C6-N1-C2	6.38	124.98	115.84
2	R	8	Y5P	N1-C2-N3	-3.61	114.73	125.33
2	Q	12	Y5P	N1-C2-N3	-3.60	114.78	125.33
2	P	12	Y5P	N1-C2-N3	-3.60	114.79	125.33
2	P	10	Y5P	N1-C2-N3	-3.59	114.80	125.33
2	Q	8	Y5P	N1-C2-N3	-3.59	114.81	125.33
2	P	8	Y5P	N1-C2-N3	-3.58	114.82	125.33
2	S	10	Y5P	N1-C2-N3	-3.58	114.85	125.33
2	Q	10	Y5P	N1-C2-N3	-3.58	114.85	125.33
2	R	10	Y5P	N1-C2-N3	-3.57	114.85	125.33
2	S	8	Y5P	N1-C2-N3	-3.57	114.85	125.33
2	O	8	Y5P	N1-C2-N3	-3.57	114.87	125.33
2	O	12	Y5P	N1-C2-N3	-3.57	114.87	125.33
2	O	10	Y5P	N1-C2-N3	-3.56	114.88	125.33
2	R	12	Y5P	N1-C2-N3	-3.56	114.89	125.33
2	P	9	Y5P	N1-C2-N3	-3.56	114.90	125.33
2	S	12	Y5P	N1-C2-N3	-3.55	114.91	125.33
2	R	9	Y5P	N1-C2-N3	-3.55	114.92	125.33
2	Q	9	Y5P	N1-C2-N3	-3.53	114.98	125.33
2	S	9	Y5P	N1-C2-N3	-3.51	115.03	125.33
2	O	9	Y5P	N1-C2-N3	-3.48	115.12	125.33
2	P	1	P5P	N1-C2-N3	-2.89	123.96	127.65
2	R	1	P5P	N1-C2-N3	-2.86	123.99	127.65
2	S	1	P5P	N1-C2-N3	-2.82	124.04	127.65
2	Q	1	P5P	N1-C2-N3	-2.81	124.06	127.65
2	O	1	P5P	N1-C2-N3	-2.80	124.07	127.65
2	O	2	Y5P	N1-C2-N3	-2.12	119.11	125.33
2	R	2	Y5P	N1-C2-N3	-2.09	119.19	125.33
2	P	2	Y5P	N1-C2-N3	-2.09	119.21	125.33
2	S	2	Y5P	N1-C2-N3	-2.08	119.24	125.33
2	Q	2	Y5P	N1-C2-N3	-2.07	119.27	125.33

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	3	P5P	O4'-C4'-C5'-O5'
2	P	3	P5P	O4'-C4'-C5'-O5'
2	Q	3	P5P	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	R	3	P5P	O4'-C4'-C5'-O5'
2	S	3	P5P	O4'-C4'-C5'-O5'
2	Q	8	Y5P	O4'-C1'-N1-C2
2	S	8	Y5P	O4'-C1'-N1-C2
2	Q	10	Y5P	O4'-C1'-N1-C2
2	R	10	Y5P	O4'-C1'-N1-C2
2	O	12	Y5P	O4'-C1'-N1-C2
2	Q	12	Y5P	O4'-C1'-N1-C2
2	O	8	Y5P	O4'-C1'-N1-C2
2	P	8	Y5P	O4'-C1'-N1-C2
2	R	8	Y5P	O4'-C1'-N1-C2
2	O	10	Y5P	O4'-C1'-N1-C2
2	P	10	Y5P	O4'-C1'-N1-C2
2	S	10	Y5P	O4'-C1'-N1-C2
2	P	12	Y5P	O4'-C1'-N1-C2
2	R	12	Y5P	O4'-C1'-N1-C2
2	S	12	Y5P	O4'-C1'-N1-C2
2	O	2	Y5P	C3'-C4'-C5'-O5'
2	P	2	Y5P	C3'-C4'-C5'-O5'
2	R	2	Y5P	C3'-C4'-C5'-O5'
2	O	3	P5P	C3'-C4'-C5'-O5'
2	P	3	P5P	C3'-C4'-C5'-O5'
2	Q	3	P5P	C3'-C4'-C5'-O5'
2	R	3	P5P	C3'-C4'-C5'-O5'
2	S	3	P5P	C3'-C4'-C5'-O5'
2	S	2	Y5P	C3'-C4'-C5'-O5'
2	S	8	Y5P	O4'-C4'-C5'-O5'
2	S	8	Y5P	C3'-C4'-C5'-O5'
2	P	2	Y5P	O4'-C1'-N1-C2
2	Q	2	Y5P	O4'-C1'-N1-C2
2	R	2	Y5P	O4'-C1'-N1-C2
2	O	2	Y5P	C4'-C5'-O5'-P
2	R	2	Y5P	C4'-C5'-O5'-P
2	Q	2	Y5P	C3'-C4'-C5'-O5'
2	R	2	Y5P	O4'-C4'-C5'-O5'
2	Q	8	Y5P	C3'-C4'-C5'-O5'
2	O	2	Y5P	O4'-C1'-N1-C2
2	P	2	Y5P	O4'-C4'-C5'-O5'
2	O	1	P5P	C4'-C5'-O5'-P
2	P	1	P5P	C4'-C5'-O5'-P
2	R	1	P5P	C4'-C5'-O5'-P
2	S	1	P5P	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
2	P	2	Y5P	C4'-C5'-O5'-P
2	Q	2	Y5P	C4'-C5'-O5'-P
2	O	2	Y5P	O4'-C4'-C5'-O5'
2	S	2	Y5P	O4'-C1'-N1-C2
2	Q	1	P5P	C4'-C5'-O5'-P
2	S	2	Y5P	C4'-C5'-O5'-P
2	S	2	Y5P	O4'-C4'-C5'-O5'
2	O	6	P5P	C4'-C5'-O5'-P
2	Q	8	Y5P	O4'-C4'-C5'-O5'
2	S	6	P5P	C4'-C5'-O5'-P
2	P	9	Y5P	O4'-C1'-N1-C2
2	Q	9	Y5P	O4'-C1'-N1-C2
2	R	9	Y5P	O4'-C1'-N1-C2
2	S	9	Y5P	O4'-C1'-N1-C2
2	Q	6	P5P	C4'-C5'-O5'-P
2	Q	6	P5P	C3'-C4'-C5'-O5'
2	S	8	Y5P	C4'-C5'-O5'-P
2	O	9	Y5P	O4'-C1'-N1-C2
2	R	3	P5P	C4'-C5'-O5'-P
2	Q	3	P5P	C4'-C5'-O5'-P
2	R	8	Y5P	C4'-C5'-O5'-P
2	R	10	Y5P	O4'-C4'-C5'-O5'
2	P	1	P5P	O4'-C4'-C5'-O5'
2	Q	8	Y5P	C4'-C5'-O5'-P
2	Q	6	P5P	O4'-C4'-C5'-O5'
2	P	10	Y5P	O4'-C4'-C5'-O5'
2	O	1	P5P	O4'-C4'-C5'-O5'
2	Q	1	P5P	O4'-C4'-C5'-O5'
2	S	1	P5P	O4'-C4'-C5'-O5'
2	R	8	Y5P	C3'-C4'-C5'-O5'
2	S	10	Y5P	O4'-C4'-C5'-O5'
2	O	9	Y5P	C2'-C1'-N1-C2
2	R	1	P5P	O4'-C4'-C5'-O5'
2	O	10	Y5P	O4'-C4'-C5'-O5'
2	Q	10	Y5P	O4'-C4'-C5'-O5'

There are no ring outliers.

28 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	4	P5P	1	0
2	R	1	P5P	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	3	P5P	1	0
2	O	8	Y5P	4	0
2	Q	11	P5P	1	0
2	Q	10	Y5P	2	0
2	P	3	P5P	1	0
2	S	11	P5P	1	0
2	R	10	Y5P	2	0
2	O	9	Y5P	1	0
2	O	1	P5P	1	0
2	O	3	P5P	1	0
2	P	8	Y5P	1	0
2	Q	1	P5P	1	0
2	R	9	Y5P	1	0
2	P	6	P5P	1	0
2	R	5	P5P	1	0
2	P	10	Y5P	2	0
2	O	11	P5P	1	0
2	O	10	Y5P	2	0
2	R	4	P5P	2	0
2	S	8	Y5P	1	0
2	O	6	P5P	1	0
2	S	10	Y5P	2	0
2	O	7	P5P	1	0
2	P	4	P5P	1	0
2	R	8	Y5P	1	0
2	Q	8	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 ⓘ

There are no chain breaks in this entry.