



## Full wwPDB EM Validation Report ⓘ

Mar 3, 2025 – 12:49 pm GMT

PDB ID : 9HBZ  
EMDB ID : EMD-52035  
Title : TiLV-NP hexamer (pseudo-C6)  
Authors : Arragain, B.; Cusack, S.  
Deposited on : 2024-11-08  
Resolution : 3.49 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](mailto: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>.

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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

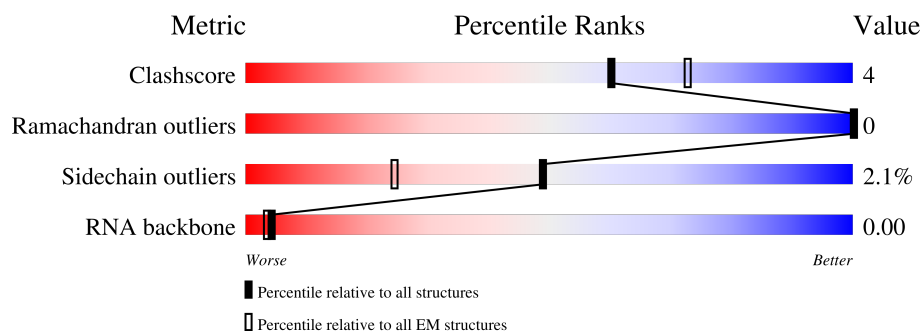
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.49 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.




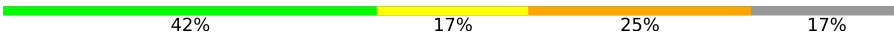
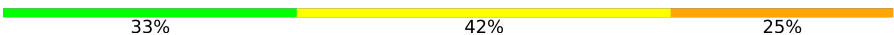

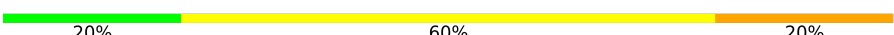
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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% 9% 12%
1	B	354	81% 7% 11%
1	C	354	77% 12% 11%
1	D	354	77% 11% 10%
1	E	354	79% 8% 12%
1	G	354	79% 8% 13%
2	F	12	42% 33% 8% 17%

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Mol	Chain	Length	Quality of chain
2	I	12	 58% 25% 17%
2	J	12	 42% 17% 25% 17%
2	O	12	 33% 42% 25%
3	H	10	 50% 30% 20%
4	K	10	 20% 60% 20%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15706 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	312	Total	C	N	O	S	0	0
			2392	1505	433	437	17		
1	C	316	Total	C	N	O	S	0	0
			2418	1519	438	444	17		
1	D	317	Total	C	N	O	S	0	0
			2422	1521	439	445	17		
1	B	314	Total	C	N	O	S	0	0
			2402	1511	435	439	17		
1	E	313	Total	C	N	O	S	1	0
			2410	1515	438	440	17		
1	G	309	Total	C	N	O	S	1	0
			2384	1501	434	432	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	12	Total	C	N	O	P	0	0
			240	116	40	72	12		
2	F	10	Total	C	N	O	P	0	0
			201	97	34	60	10		
2	I	12	Total	C	N	O	P	0	0
			240	116	40	72	12		
2	J	10	Total	C	N	O	P	0	0
			201	97	34	60	10		

- Molecule 3 is a RNA chain called 40-mer vRNA loop.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	10	Total	C	N	O	P	0	0
			198	96	32	60	10		


- Molecule 4 is a RNA chain called 40-mer vRNA loop.

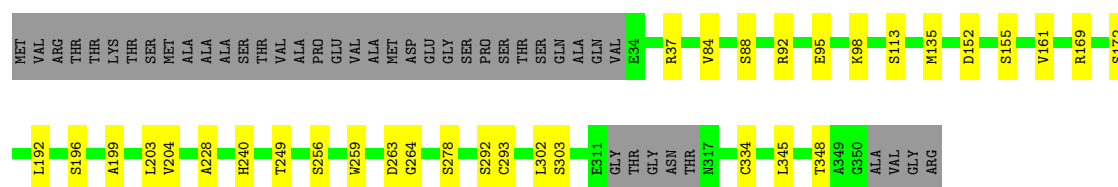
Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	10	Total	C	N	O	P	0	0
			198	96	32	60	10		

### 3 Residue-property plots

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.

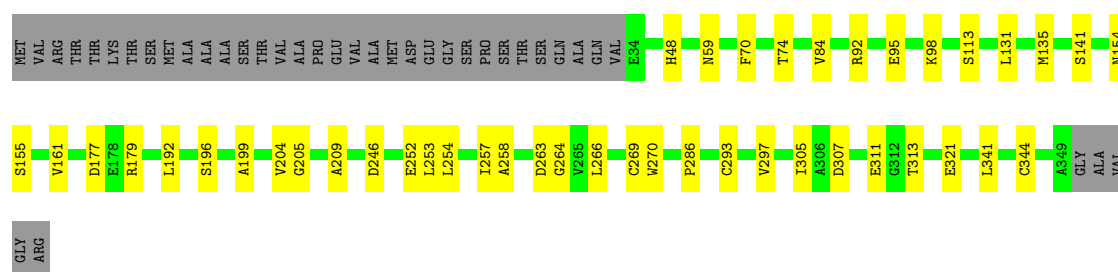
- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)

Chain A: 




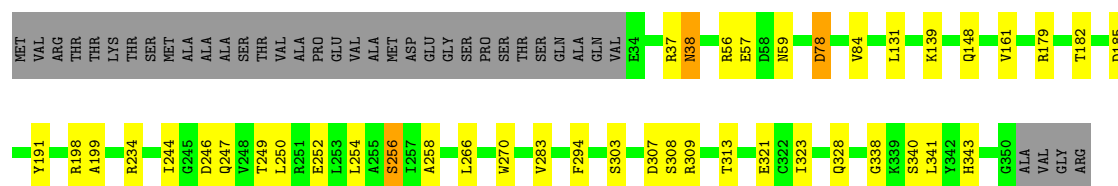
- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)

Chain C: 




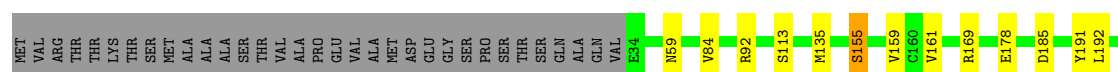
- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)

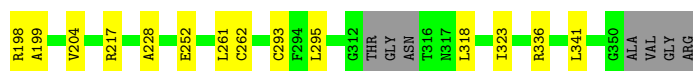
Chain D: 



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

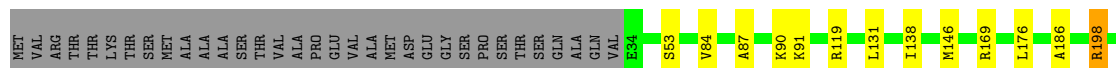
Chain B: 





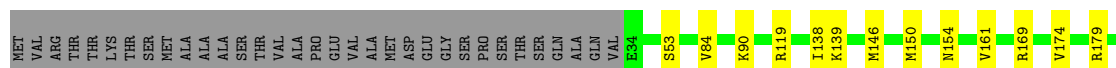
- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)

Chain E: 79% 8% 12%



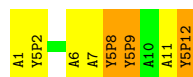
- Molecule 1: Tilapia Lake Virus nucleoprotein (segment 4)

Chain G: 79% 8% 13%



- Molecule 2: 40-mer vRNA loop

Chain O: 33% 42% 25%



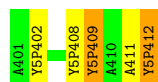
- Molecule 2: 40-mer vRNA loop

Chain F: 42% 33% 8% 17%



- Molecule 2: 40-mer vRNA loop

Chain I: 58% 25% 17%

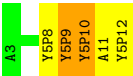


- Molecule 2: 40-mer vRNA loop

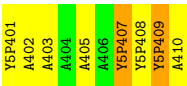
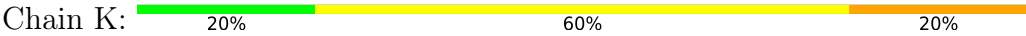
Chain J: 42% 17% 25% 17%



- Molecule 3: 40-mer vRNA loop



- Molecule 4: 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	151178	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: Y5P, P5P

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	0.24	0/2433	0.47	0/3276
1	B	0.24	0/2442	0.47	0/3287
1	C	0.25	0/2460	0.49	0/3315
1	D	0.24	0/2464	0.48	0/3320
1	E	0.24	0/2450	0.47	0/3297
1	G	0.24	0/2424	0.47	0/3262
All	All	0.24	0/14673	0.48	0/19757

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	2392	0	2430	20	0
1	B	2402	0	2436	17	0
1	C	2418	0	2454	25	0
1	D	2422	0	2457	34	0
1	E	2410	0	2448	28	0
1	G	2384	0	2427	22	0
2	F	201	0	107	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	240	0	129	3	0
2	J	201	0	107	4	0
2	O	240	0	129	5	0
3	H	198	0	109	3	0
4	K	198	0	109	6	0
All	All	15706	0	15342	134	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 (134) 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:E:340:SER:OG	1:G:295:LEU:O	1.96	0.83
1:D:179:ARG:NH1	1:E:217:ARG:O	2.12	0.82
1:C:59:ASN:ND2	1:C:252:GLU:OE2	2.17	0.77
1:A:169:ARG:NH1	1:A:256:SER:O	2.18	0.77
1:D:340:SER:OG	1:E:295:LEU:O	2.02	0.77
1:D:338:GLY:O	1:E:308:SER:OG	2.02	0.76
1:E:91:LYS:NZ	3:H:11:P5P:OP1	2.22	0.72
1:D:198:ARG:NE	2:O:8:Y5P:O2'	2.27	0.68
1:G:227:THR:O	1:G:288:GLN:NE2	2.26	0.67
1:D:59:ASN:ND2	1:D:252:GLU:OE1	2.28	0.66
1:D:321:GLU:OE2	1:E:303:SER:OG	2.16	0.64
1:C:321:GLU:OE2	1:D:303:SER:OG	2.11	0.63
1:A:259:TRP:CZ2	1:C:297:VAL:HG21	2.34	0.63
1:D:244:ILE:HG21	1:D:328:GLN:HG3	1.81	0.63
1:D:252:GLU:O	1:D:256:SER:OG	2.17	0.62
1:C:258:ALA:HB2	1:C:266:LEU:HD13	1.82	0.61
1:B:161:VAL:HG21	1:B:199:ALA:HB3	1.83	0.61
1:A:113:SER:O	1:A:113:SER:OG	2.19	0.60
1:E:254:LEU:HD13	1:E:341:LEU:HD22	1.83	0.59
1:B:217:ARG:O	1:G:179:ARG:NH1	2.36	0.59
1:C:258:ALA:CB	1:C:266:LEU:HD13	2.33	0.58
1:G:208:PHE:CD1	4:K:409:Y5P:H4A	2.39	0.57
1:C:253:LEU:HD23	1:C:270:TRP:HB2	1.87	0.57
1:D:139:LYS:NZ	2:O:6:P5P:OP2	2.36	0.55
1:B:59:ASN:ND2	1:B:252:GLU:OE2	2.40	0.55
1:E:264:GLY:N	1:E:339:LYS:O	2.39	0.55
1:D:307:ASP:OD1	1:D:309:ARG:N	2.40	0.54
1:E:131:LEU:HD11	3:H:9:Y5P:O4'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:VAL:HG12	1:D:84:VAL:O	2.07	0.54
1:A:263:ASP:OD1	1:A:264:GLY:N	2.41	0.54
1:G:268:GLU:N	1:G:268:GLU:OE1	2.41	0.54
1:B:113:SER:O	1:B:113:SER:OG	2.21	0.53
1:C:113:SER:OG	1:C:113:SER:O	2.24	0.53
1:D:323:ILE:HG23	1:E:302:LEU:HD21	1.89	0.53
1:A:196:SER:O	1:A:204:VAL:HG21	2.08	0.53
1:E:261:LEU:HB3	1:G:297:VAL:HG13	1.91	0.53
1:D:185:ASP:O	1:D:191:TYR:OH	2.25	0.52
1:D:313:THR:HG22	1:D:313:THR:O	2.10	0.52
1:C:131:LEU:HD11	2:J:407:Y5P:O4'	2.09	0.52
1:A:293:CYS:SG	1:B:261:LEU:HD21	2.50	0.52
2:O:12:Y5P:O5'	2:O:12:Y5P:H6	2.10	0.51
1:A:84:VAL:HG13	1:A:92:ARG:HG3	1.93	0.51
1:E:268:GLU:N	1:E:268:GLU:OE1	2.44	0.51
1:D:258:ALA:HB2	1:D:266:LEU:HD13	1.91	0.50
1:C:95:GLU:OE1	1:C:98:LYS:NZ	2.44	0.50
1:D:307:ASP:OD2	1:D:309:ARG:NH2	2.36	0.50
1:D:254:LEU:HD13	1:D:341:LEU:HD22	1.94	0.50
1:C:254:LEU:HD13	1:C:341:LEU:HD22	1.94	0.50
1:B:295:LEU:O	1:G:340:SER:OG	2.29	0.50
1:G:150:MET:HE3	4:K:407:Y5P:H4A	1.93	0.50
1:D:258:ALA:CB	1:D:266:LEU:HD13	2.41	0.49
1:G:84:VAL:HG12	1:G:84:VAL:O	2.13	0.49
1:C:253:LEU:HD21	1:C:269:CYS:HB2	1.95	0.49
1:G:150:MET:CE	4:K:407:Y5P:H4A	2.42	0.49
1:B:185:ASP:O	1:B:191:TYR:OH	2.27	0.49
1:A:303:SER:O	1:B:336:ARG:NH2	2.46	0.48
1:C:192:LEU:HD12	1:C:204:VAL:HG22	1.95	0.48
1:E:254:LEU:O	1:E:258:ALA:N	2.47	0.48
1:A:302:LEU:HD21	1:B:323:ILE:HG23	1.96	0.48
1:E:84:VAL:O	1:E:84:VAL:HG12	2.13	0.48
1:E:169:ARG:NH1	1:E:228:ALA:O	2.39	0.48
1:C:263:ASP:OD1	1:C:264:GLY:N	2.47	0.48
1:E:138:ILE:HD12	1:E:146:MET:HG2	1.96	0.47
1:C:84:VAL:HG13	1:C:92:ARG:HG3	1.96	0.47
1:G:139:LYS:NZ	4:K:405:P5P:OP2	2.39	0.47
1:B:169:ARG:NH1	1:B:228:ALA:O	2.43	0.47
1:B:262:CYS:O	1:B:341:LEU:N	2.45	0.47
1:D:37:ARG:NH2	1:D:148:GLN:OE1	2.48	0.46
1:C:257:ILE:HD12	1:C:286:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:THR:O	1:D:185:ASP:N	2.48	0.46
1:A:249:THR:HG23	1:A:278:SER:O	2.16	0.46
1:B:84:VAL:HG13	1:B:92:ARG:HG3	1.98	0.46
1:E:198[B]:ARG:HH11	3:H:10:Y5P:H5	1.81	0.46
1:E:261:LEU:O	1:G:297:VAL:HG22	2.16	0.46
1:A:84:VAL:O	1:A:84:VAL:HG12	2.16	0.46
1:C:177:ASP:OD2	1:C:179:ARG:NE	2.44	0.46
1:C:305:ILE:HG22	1:C:307:ASP:H	1.81	0.46
1:D:343:HIS:NE2	1:E:293:CYS:O	2.48	0.46
2:F:12:Y5P:H6	2:F:12:Y5P:O5'	2.16	0.46
1:A:161:VAL:HG21	1:A:199:ALA:HB3	1.99	0.45
1:C:84:VAL:HG12	1:C:84:VAL:O	2.16	0.45
1:G:321:GLU:OE1	1:G:336:ARG:NH1	2.49	0.45
1:E:343:HIS:NE2	1:G:293:CYS:O	2.43	0.45
1:A:303:SER:HG	1:B:318:LEU:HD22	1.80	0.45
1:B:84:VAL:HG12	1:B:84:VAL:O	2.17	0.45
1:A:345:LEU:HA	1:A:348:THR:HG22	1.99	0.45
1:C:70:PHE:O	1:C:74:THR:OG1	2.26	0.45
2:O:6:P5P:H3'	2:O:7:P5P:H8	1.98	0.45
2:J:404:P5P:C2'	2:J:405:P5P:O5'	2.65	0.45
1:G:154:ASN:OD1	4:K:407:Y5P:N3	2.50	0.45
1:G:254:LEU:HD13	1:G:341:LEU:HD22	2.00	0.44
1:D:321:GLU:CD	1:E:303:SER:HG	2.20	0.44
1:C:313:THR:HG22	1:C:313:THR:O	2.16	0.44
1:D:78:ASP:N	1:D:78:ASP:OD1	2.51	0.43
1:D:234:ARG:NH2	1:D:247:GLN:O	2.51	0.43
1:G:169:ARG:NH1	1:G:228:ALA:O	2.45	0.43
1:B:198:ARG:NH1	2:F:7:P5P:O2'	2.52	0.42
1:C:84:VAL:CG1	1:C:92:ARG:HE	2.32	0.42
1:D:182:THR:N	1:D:185:ASP:OD2	2.52	0.42
1:G:174:VAL:HG22	1:G:251:ARG:NH2	2.33	0.42
1:D:38:ASN:N	1:D:38:ASN:OD1	2.52	0.42
1:D:161:VAL:HG21	1:D:199:ALA:HB3	2.01	0.42
2:F:6:P5P:C2'	2:F:7:P5P:O5'	2.68	0.42
1:A:95:GLU:OE1	1:A:98:LYS:NZ	2.52	0.42
1:E:254:LEU:CD1	1:E:341:LEU:HD22	2.50	0.42
1:A:84:VAL:H	2:I:409:Y5P:H6	1.84	0.42
1:A:203:LEU:CD2	1:A:228:ALA:HB3	2.49	0.42
1:D:249:THR:HG22	1:D:250:LEU:N	2.35	0.42
1:D:283:VAL:O	1:D:283:VAL:HG12	2.20	0.42
1:B:155:SER:O	1:B:159:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:LEU:HD11	1:E:342:TYR:CE2	2.55	0.42
1:D:250:LEU:HD13	1:D:270:TRP:CE3	2.55	0.41
2:F:7:P5P:OP2	2:F:7:P5P:H8	2.19	0.41
2:I:412:Y5P:H6	2:I:412:Y5P:O5'	2.19	0.41
2:J:410:Y5P:H6	2:J:410:Y5P:O5'	2.20	0.41
1:D:56:ARG:O	1:D:56:ARG:HG2	2.20	0.41
1:D:131:LEU:HD11	2:O:9:Y5P:O4'	2.20	0.41
1:C:161:VAL:HG21	1:C:199:ALA:HB3	2.03	0.41
1:C:205:GLY:HA2	1:C:209:ALA:HB2	2.02	0.41
1:E:186:ALA:HB1	1:G:297:VAL:HG11	2.01	0.41
1:A:88:SER:OG	2:I:412:Y5P:OP1	2.33	0.41
1:B:192:LEU:HD12	1:B:204:VAL:HG22	2.03	0.41
1:E:176:LEU:HD13	1:G:293:CYS:HB3	2.02	0.41
1:A:192:LEU:HD12	1:A:204:VAL:HG22	2.01	0.41
1:G:138:ILE:HD12	1:G:146:MET:HG2	2.02	0.41
1:E:87:ALA:HB1	1:E:91:LYS:CG	2.50	0.41
1:E:84:VAL:O	1:E:84:VAL:CG1	2.69	0.40
1:A:37:ARG:NH1	1:A:152:ASP:OD2	2.53	0.40
1:C:154:ASN:OD1	2:J:406:Y5P:N3	2.55	0.40
1:D:294:PHE:O	1:D:308:SER:OG	2.36	0.40
4:K:402:P5P:H2'	4:K:403:P5P:O4'	2.21	0.40
1:G:161:VAL:HG21	1:G:199:ALA:HB3	2.04	0.40
1:C:196:SER:O	1:C:204:VAL:HG21	2.22	0.40
1:E:345:LEU:HA	1:E:348:THR:HG22	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	308/354 (87%)	303 (98%)	5 (2%)	0	<a href="#">100</a> <a href="#">100</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	308/354 (87%)	305 (99%)	3 (1%)	0	100	100
1	C	314/354 (89%)	302 (96%)	12 (4%)	0	100	100
1	D	315/354 (89%)	306 (97%)	9 (3%)	0	100	100
1	E	308/354 (87%)	305 (99%)	3 (1%)	0	100	100
1	G	304/354 (86%)	303 (100%)	1 (0%)	0	100	100
All	All	1857/2124 (87%)	1824 (98%)	33 (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	253/285 (89%)	247 (98%)	6 (2%)	44	68
1	B	253/285 (89%)	249 (98%)	4 (2%)	58	76
1	C	256/285 (90%)	248 (97%)	8 (3%)	35	63
1	D	256/285 (90%)	251 (98%)	5 (2%)	50	72
1	E	255/285 (90%)	249 (98%)	6 (2%)	44	68
1	G	252/285 (88%)	247 (98%)	5 (2%)	50	72
All	All	1525/1710 (89%)	1491 (98%)	34 (2%)	49	70

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	MET
1	A	155	SER
1	A	172	SER
1	A	240	HIS
1	A	292	SER
1	A	334	CYS
1	C	48	HIS
1	C	135	MET

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Mol	Chain	Res	Type
1	C	141	SER
1	C	155	SER
1	C	246	ASP
1	C	293	CYS
1	C	311	GLU
1	C	344	CYS
1	D	38	ASN
1	D	57	GLU
1	D	78	ASP
1	D	246	ASP
1	D	256	SER
1	B	135	MET
1	B	155	SER
1	B	178	GLU
1	B	293	CYS
1	E	53	SER
1	E	90	LYS
1	E	119	ARG
1	E	198[A]	ARG
1	E	198[B]	ARG
1	E	293	CYS
1	G	53	SER
1	G	90	LYS
1	G	119	ARG
1	G	198[A]	ARG
1	G	198[B]	ARG

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

Mol	Chain	Res	Type
1	C	240	HIS
1	D	240	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	0/12	-	-
2	I	0/12	-	-
2	J	0/12	-	-
2	O	0/12	-	-

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	H	0/10	-	-
4	K	0/10	-	-
All	All	0/68	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

64 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	O	1	2	16,23,24	0.79	0	14,33,36	0.79	1 (7%)
2	Y5P	J	410	2	14,19,20	2.35	1 (7%)	18,26,29	0.99	1 (5%)
3	Y5P	H	8	3	14,19,20	2.32	1 (7%)	18,26,29	0.99	1 (5%)
3	Y5P	H	12	3	14,19,20	2.31	1 (7%)	18,26,29	1.02	1 (5%)
2	P5P	I	405	2	16,23,24	0.80	0	14,33,36	0.74	0
3	Y5P	H	10	3	14,19,20	2.34	1 (7%)	18,26,29	1.00	1 (5%)
2	P5P	I	401	2	16,23,24	0.77	0	14,33,36	0.74	0
2	P5P	O	4	2	16,23,24	0.79	0	14,33,36	0.73	0
4	Y5P	K	408	4	14,19,20	2.37	1 (7%)	18,26,29	0.99	1 (5%)
2	P5P	O	5	2	16,23,24	0.78	0	14,33,36	0.75	0
4	Y5P	K	401	4	14,19,20	2.32	1 (7%)	18,26,29	1.00	1 (5%)
2	P5P	I	403	2	16,23,24	0.78	0	14,33,36	0.73	0
2	P5P	F	10	2	16,23,24	0.79	0	14,33,36	0.76	0
2	P5P	O	7	2	16,23,24	0.78	0	14,33,36	0.74	0
2	Y5P	I	408	2	14,19,20	2.37	1 (7%)	18,26,29	0.98	1 (5%)
2	P5P	I	410	2	16,23,24	0.79	0	14,33,36	0.77	0
4	P5P	K	404	4	16,23,24	0.78	0	14,33,36	0.74	0
2	P5P	F	5	2	16,23,24	0.78	0	14,33,36	0.76	0
3	Y5P	H	9	3	14,19,20	2.37	1 (7%)	18,26,29	0.99	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	P5P	O	10	2	16,23,24	0.76	0	14,33,36	0.74	0
2	P5P	J	404	2	16,23,24	0.79	0	14,33,36	0.76	0
3	P5P	H	3	3	16,23,24	0.77	0	14,33,36	0.74	0
4	P5P	K	402	4	16,23,24	0.78	0	14,33,36	0.72	0
3	P5P	H	11	3	16,23,24	0.79	0	14,33,36	0.75	0
4	Y5P	K	409	4	14,19,20	2.34	1 (7%)	18,26,29	0.98	1 (5%)
2	Y5P	O	12	2	14,19,20	2.29	1 (7%)	18,26,29	0.99	1 (5%)
2	P5P	I	411	2	16,23,24	0.77	0	14,33,36	0.74	1 (7%)
2	Y5P	F	12	2	14,19,20	2.33	1 (7%)	18,26,29	0.99	1 (5%)
2	P5P	I	406	2	16,23,24	0.78	0	14,33,36	0.74	0
2	P5P	F	7	2	16,23,24	0.78	0	14,33,36	0.73	0
2	Y5P	I	409	2	14,19,20	2.37	1 (7%)	18,26,29	0.99	1 (5%)
2	P5P	J	408	2	16,23,24	0.77	0	14,33,36	0.78	0
2	P5P	J	403	2	16,23,24	0.77	0	14,33,36	0.76	0
2	P5P	O	3	2	16,23,24	0.80	0	14,33,36	0.74	0
3	P5P	H	7	3	16,23,24	0.78	0	14,33,36	0.73	0
2	Y5P	F	9	2	14,19,20	2.33	1 (7%)	18,26,29	1.02	1 (5%)
3	P5P	H	6	3	16,23,24	0.77	0	14,33,36	0.81	0
2	P5P	I	407	2	16,23,24	0.78	0	14,33,36	0.74	0
2	P5P	J	409	2	16,23,24	0.80	0	14,33,36	0.73	0
2	Y5P	F	8	2	14,19,20	2.33	1 (7%)	18,26,29	0.99	1 (5%)
4	P5P	K	410	4	16,23,24	0.77	0	14,33,36	0.73	1 (7%)
2	P5P	O	11	2	16,23,24	0.78	1 (6%)	14,33,36	0.87	0
2	P5P	O	6	2	16,23,24	0.79	0	14,33,36	0.76	0
2	P5P	F	4	2	16,23,24	0.78	0	14,33,36	0.76	0
2	P5P	J	401	2	16,23,24	0.79	0	14,33,36	0.73	0
2	P5P	F	11	2	16,23,24	0.77	0	14,33,36	0.73	0
2	Y5P	O	8	2	14,19,20	2.39	1 (7%)	18,26,29	0.99	1 (5%)
2	P5P	F	6	2	16,23,24	0.79	0	14,33,36	0.76	0
2	Y5P	O	2	2	14,19,20	2.30	1 (7%)	18,26,29	1.00	1 (5%)
2	Y5P	J	406	2	14,19,20	2.35	1 (7%)	18,26,29	0.98	1 (5%)
2	Y5P	J	407	2	14,19,20	2.30	1 (7%)	18,26,29	1.02	1 (5%)
2	Y5P	I	412	2	14,19,20	2.30	1 (7%)	18,26,29	0.99	1 (5%)
2	P5P	I	404	2	16,23,24	0.79	0	14,33,36	0.73	0
2	P5P	J	405	2	16,23,24	0.77	0	14,33,36	0.73	0
2	P5P	F	3	2	16,23,24	0.77	0	14,33,36	0.74	0
3	P5P	H	4	3	16,23,24	0.79	0	14,33,36	0.73	0
4	P5P	K	405	4	16,23,24	0.77	0	14,33,36	0.77	0
4	Y5P	K	407	4	14,19,20	2.31	1 (7%)	18,26,29	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	P5P	K	403	4	16,23,24	0.79	0	14,33,36	0.75	0
2	Y5P	O	9	2	14,19,20	2.35	1 (7%)	18,26,29	1.01	1 (5%)
2	Y5P	I	402	2	14,19,20	2.38	1 (7%)	18,26,29	0.98	1 (5%)
4	P5P	K	406	4	16,23,24	0.79	0	14,33,36	0.73	0
3	P5P	H	5	3	16,23,24	0.79	0	14,33,36	0.74	0
2	P5P	J	402	2	16,23,24	0.78	0	14,33,36	0.76	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	P5P	O	1	2	-	2/3/25/26	0/3/3/3
2	Y5P	J	410	2	-	1/7/33/34	0/2/2/2
3	Y5P	H	8	3	-	3/7/33/34	0/2/2/2
3	Y5P	H	12	3	-	1/7/33/34	0/2/2/2
2	P5P	I	405	2	-	0/3/25/26	0/3/3/3
3	Y5P	H	10	3	-	2/7/33/34	0/2/2/2
2	P5P	I	401	2	-	0/3/25/26	0/3/3/3
2	P5P	O	4	2	-	0/3/25/26	0/3/3/3
4	Y5P	K	408	4	-	1/7/33/34	0/2/2/2
2	P5P	O	5	2	-	0/3/25/26	0/3/3/3
4	Y5P	K	401	4	-	4/7/33/34	0/2/2/2
2	P5P	I	403	2	-	0/3/25/26	0/3/3/3
2	P5P	F	10	2	-	1/3/25/26	0/3/3/3
2	P5P	O	7	2	-	0/3/25/26	0/3/3/3
2	Y5P	I	408	2	-	2/7/33/34	0/2/2/2
2	P5P	I	410	2	-	2/3/25/26	0/3/3/3
4	P5P	K	404	4	-	0/3/25/26	0/3/3/3
2	P5P	F	5	2	-	2/3/25/26	0/3/3/3
3	Y5P	H	9	3	-	1/7/33/34	0/2/2/2
2	P5P	O	10	2	-	1/3/25/26	0/3/3/3
2	P5P	J	404	2	-	0/3/25/26	0/3/3/3
3	P5P	H	3	3	-	3/3/25/26	0/3/3/3
4	P5P	K	402	4	-	3/3/25/26	0/3/3/3
3	P5P	H	11	3	-	0/3/25/26	0/3/3/3
4	Y5P	K	409	4	-	2/7/33/34	0/2/2/2
2	Y5P	O	12	2	-	1/7/33/34	0/2/2/2
2	P5P	I	411	2	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y5P	F	12	2	-	1/7/33/34	0/2/2/2
2	P5P	I	406	2	-	0/3/25/26	0/3/3/3
2	P5P	F	7	2	-	1/3/25/26	0/3/3/3
2	Y5P	I	409	2	-	1/7/33/34	0/2/2/2
2	P5P	J	408	2	-	1/3/25/26	0/3/3/3
2	P5P	J	403	2	-	2/3/25/26	0/3/3/3
2	P5P	O	3	2	-	2/3/25/26	0/3/3/3
3	P5P	H	7	3	-	0/3/25/26	0/3/3/3
2	Y5P	F	9	2	-	1/7/33/34	0/2/2/2
3	P5P	H	6	3	-	1/3/25/26	0/3/3/3
2	P5P	I	407	2	-	2/3/25/26	0/3/3/3
2	P5P	J	409	2	-	0/3/25/26	0/3/3/3
2	Y5P	F	8	2	-	3/7/33/34	0/2/2/2
4	P5P	K	410	4	-	0/3/25/26	0/3/3/3
2	P5P	O	11	2	-	0/3/25/26	0/3/3/3
2	P5P	O	6	2	-	0/3/25/26	0/3/3/3
2	P5P	F	4	2	-	0/3/25/26	0/3/3/3
2	P5P	J	401	2	-	0/3/25/26	0/3/3/3
2	P5P	F	11	2	-	0/3/25/26	0/3/3/3
2	Y5P	O	8	2	-	2/7/33/34	0/2/2/2
2	P5P	F	6	2	-	0/3/25/26	0/3/3/3
2	Y5P	O	2	2	-	3/7/33/34	0/2/2/2
2	Y5P	J	406	2	-	3/7/33/34	0/2/2/2
2	Y5P	J	407	2	-	1/7/33/34	0/2/2/2
2	Y5P	I	412	2	-	1/7/33/34	0/2/2/2
2	P5P	I	404	2	-	0/3/25/26	0/3/3/3
2	P5P	J	405	2	-	1/3/25/26	0/3/3/3
2	P5P	F	3	2	-	0/3/25/26	0/3/3/3
3	P5P	H	4	3	-	0/3/25/26	0/3/3/3
4	P5P	K	405	4	-	1/3/25/26	0/3/3/3
4	Y5P	K	407	4	-	3/7/33/34	0/2/2/2
4	P5P	K	403	4	-	0/3/25/26	0/3/3/3
2	Y5P	O	9	2	-	1/7/33/34	0/2/2/2
2	Y5P	I	402	2	-	1/7/33/34	0/2/2/2
4	P5P	K	406	4	-	0/3/25/26	0/3/3/3
3	P5P	H	5	3	-	0/3/25/26	0/3/3/3
2	P5P	J	402	2	-	2/3/25/26	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	8	Y5P	C4-N3	-8.77	1.38	1.46
2	I	402	Y5P	C4-N3	-8.75	1.38	1.46
3	H	9	Y5P	C4-N3	-8.73	1.38	1.46
4	K	408	Y5P	C4-N3	-8.72	1.38	1.46
2	I	408	Y5P	C4-N3	-8.72	1.38	1.46
2	I	409	Y5P	C4-N3	-8.72	1.38	1.46
2	O	9	Y5P	C4-N3	-8.65	1.38	1.46
2	J	410	Y5P	C4-N3	-8.63	1.38	1.46
2	J	406	Y5P	C4-N3	-8.60	1.38	1.46
3	H	10	Y5P	C4-N3	-8.60	1.38	1.46
4	K	409	Y5P	C4-N3	-8.60	1.38	1.46
2	F	12	Y5P	C4-N3	-8.57	1.38	1.46
2	F	9	Y5P	C4-N3	-8.55	1.38	1.46
4	K	401	Y5P	C4-N3	-8.54	1.38	1.46
2	F	8	Y5P	C4-N3	-8.53	1.38	1.46
3	H	8	Y5P	C4-N3	-8.53	1.38	1.46
3	H	12	Y5P	C4-N3	-8.49	1.38	1.46
2	O	2	Y5P	C4-N3	-8.48	1.38	1.46
4	K	407	Y5P	C4-N3	-8.48	1.38	1.46
2	J	407	Y5P	C4-N3	-8.46	1.38	1.46
2	I	412	Y5P	C4-N3	-8.44	1.38	1.46
2	O	12	Y5P	C4-N3	-8.42	1.38	1.46
2	O	11	P5P	C8-N7	-2.02	1.31	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	407	Y5P	N1-C2-N3	-3.62	114.73	125.33
3	H	12	Y5P	N1-C2-N3	-3.61	114.74	125.33
2	O	12	Y5P	N1-C2-N3	-3.60	114.78	125.33
3	H	8	Y5P	N1-C2-N3	-3.59	114.81	125.33
3	H	10	Y5P	N1-C2-N3	-3.58	114.83	125.33
2	O	2	Y5P	N1-C2-N3	-3.58	114.83	125.33
2	F	12	Y5P	N1-C2-N3	-3.58	114.84	125.33
2	F	8	Y5P	N1-C2-N3	-3.58	114.84	125.33
2	I	412	Y5P	N1-C2-N3	-3.57	114.85	125.33
2	J	407	Y5P	N1-C2-N3	-3.57	114.88	125.33
2	O	8	Y5P	N1-C2-N3	-3.55	114.91	125.33
4	K	401	Y5P	N1-C2-N3	-3.55	114.91	125.33
2	F	9	Y5P	N1-C2-N3	-3.55	114.93	125.33
4	K	409	Y5P	N1-C2-N3	-3.54	114.94	125.33
2	J	410	Y5P	N1-C2-N3	-3.54	114.95	125.33
2	J	406	Y5P	N1-C2-N3	-3.53	114.98	125.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	408	Y5P	N1-C2-N3	-3.53	114.98	125.33
3	H	9	Y5P	N1-C2-N3	-3.53	114.98	125.33
2	O	9	Y5P	N1-C2-N3	-3.52	115.00	125.33
4	K	408	Y5P	N1-C2-N3	-3.52	115.01	125.33
2	I	402	Y5P	N1-C2-N3	-3.51	115.04	125.33
2	I	409	Y5P	N1-C2-N3	-3.48	115.13	125.33
2	I	411	P5P	C6-N1-C2	2.07	118.80	115.84
2	O	1	P5P	C6-N1-C2	2.03	118.74	115.84
4	K	410	P5P	C6-N1-C2	2.00	118.71	115.84

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	402	Y5P	O4'-C1'-N1-C2
2	O	3	P5P	O4'-C4'-C5'-O5'
2	F	8	Y5P	O4'-C1'-N1-C2
2	J	406	Y5P	O4'-C1'-N1-C2
2	O	12	Y5P	O4'-C1'-N1-C2
3	H	8	Y5P	O4'-C1'-N1-C2
3	H	12	Y5P	O4'-C1'-N1-C2
4	K	402	P5P	O4'-C4'-C5'-O5'
2	O	8	Y5P	O4'-C1'-N1-C2
2	I	408	Y5P	O4'-C1'-N1-C2
2	F	12	Y5P	O4'-C1'-N1-C2
2	J	410	Y5P	O4'-C1'-N1-C2
4	K	407	Y5P	O4'-C1'-N1-C2
4	K	409	Y5P	O4'-C1'-N1-C2
2	O	3	P5P	C3'-C4'-C5'-O5'
4	K	402	P5P	C3'-C4'-C5'-O5'
3	H	3	P5P	O4'-C4'-C5'-O5'
3	H	10	Y5P	O4'-C1'-N1-C2
2	O	2	Y5P	O4'-C1'-N1-C2
2	I	412	Y5P	O4'-C1'-N1-C2
4	K	401	Y5P	O4'-C1'-N1-C2
3	H	3	P5P	C3'-C4'-C5'-O5'
4	K	401	Y5P	C3'-C4'-C5'-O5'
2	O	2	Y5P	C4'-C5'-O5'-P
2	F	8	Y5P	C3'-C4'-C5'-O5'
3	H	8	Y5P	C3'-C4'-C5'-O5'
2	O	1	P5P	C4'-C5'-O5'-P
2	J	406	Y5P	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	J	403	P5P	C3'-C4'-C5'-O5'
4	K	407	Y5P	C3'-C4'-C5'-O5'
2	F	8	Y5P	O4'-C4'-C5'-O5'
2	J	405	P5P	C4'-C5'-O5'-P
4	K	401	Y5P	C4'-C5'-O5'-P
4	K	405	P5P	C4'-C5'-O5'-P
2	I	410	P5P	O4'-C4'-C5'-O5'
2	F	9	Y5P	O4'-C1'-N1-C6
2	J	407	Y5P	O4'-C1'-N1-C6
2	F	7	P5P	C4'-C5'-O5'-P
2	O	2	Y5P	C3'-C4'-C5'-O5'
2	J	402	P5P	C3'-C4'-C5'-O5'
2	F	5	P5P	C3'-C4'-C5'-O5'
3	H	8	Y5P	O4'-C4'-C5'-O5'
2	I	409	Y5P	O4'-C1'-N1-C6
3	H	6	P5P	C4'-C5'-O5'-P
2	J	403	P5P	O4'-C4'-C5'-O5'
2	J	406	Y5P	O4'-C4'-C5'-O5'
4	K	407	Y5P	O4'-C4'-C5'-O5'
3	H	9	Y5P	O4'-C1'-N1-C2
4	K	408	Y5P	O4'-C1'-N1-C2
4	K	402	P5P	C4'-C5'-O5'-P
2	O	9	Y5P	O4'-C1'-N1-C2
2	O	8	Y5P	C3'-C4'-C5'-O5'
2	I	407	P5P	C4'-C5'-O5'-P
2	O	1	P5P	O4'-C4'-C5'-O5'
3	H	10	Y5P	O4'-C4'-C5'-O5'
4	K	409	Y5P	O4'-C4'-C5'-O5'
2	J	402	P5P	O4'-C4'-C5'-O5'
2	F	5	P5P	O4'-C4'-C5'-O5'
2	I	408	Y5P	C3'-C4'-C5'-O5'
2	F	10	P5P	O4'-C4'-C5'-O5'
2	J	408	P5P	O4'-C4'-C5'-O5'
2	O	10	P5P	O4'-C4'-C5'-O5'
4	K	401	Y5P	O4'-C4'-C5'-O5'
3	H	3	P5P	C4'-C5'-O5'-P
2	I	407	P5P	O4'-C4'-C5'-O5'
2	I	410	P5P	C3'-C4'-C5'-O5'

There are no ring outliers.

23 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	410	Y5P	1	0
3	H	10	Y5P	1	0
2	O	7	P5P	1	0
3	H	9	Y5P	1	0
2	J	404	P5P	1	0
4	K	402	P5P	1	0
3	H	11	P5P	1	0
4	K	409	Y5P	1	0
2	O	12	Y5P	1	0
2	F	12	Y5P	1	0
2	F	7	P5P	3	0
2	I	409	Y5P	1	0
2	O	6	P5P	2	0
2	O	8	Y5P	1	0
2	F	6	P5P	1	0
2	J	406	Y5P	1	0
2	J	407	Y5P	1	0
2	I	412	Y5P	2	0
2	J	405	P5P	1	0
4	K	405	P5P	1	0
4	K	407	Y5P	3	0
4	K	403	P5P	1	0
2	O	9	Y5P	1	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
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	291:GLY	C	292:SER	N	3.24