



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 20, 2020 – 09:47 AM EST

PDB ID : 6VBW  
EMDB ID: : EMD-21146  
Title : Cryo-EM structure of Cascade-TniQ-dsDNA ternary complex  
Authors : Jia, N.; Patel, D.J.  
Deposited on : 2019-12-19  
Resolution : 3.20 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB 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.

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MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

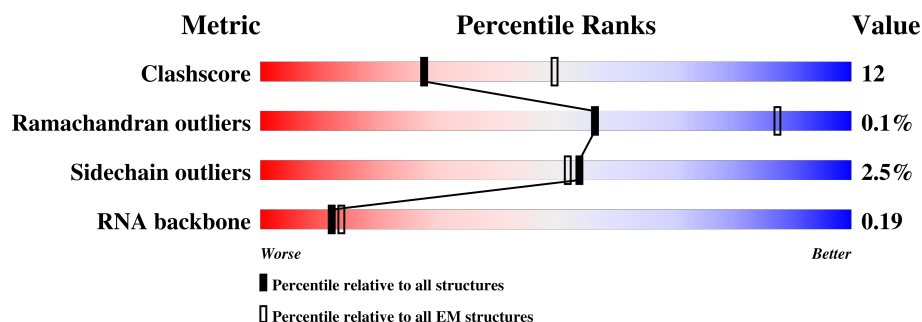
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	M	22	23% 9% 68%
2	L	100	31% 8% 61%
3	K	61	28% 43% 30%
4	A	640	50% 19% . 30%
5	B	352	77% 18% .
5	C	352	79% 16% . .
5	D	352	78% 17% . .
5	E	352	78% 18% . .

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Mol	Chain	Length	Quality of chain
5	F	352	<div><div></div><div>78%</div><div>18%</div><div>••</div></div>
5	G	352	<div><div></div><div>66%</div><div>19%</div><div>•13%</div></div>
6	H	199	<div><div></div><div>52%</div><div>15%</div><div>•32%</div></div>
7	I	394	<div><div></div><div>77%</div><div>18%</div><div>5%</div></div>
7	J	394	<div><div></div><div>79%</div><div>17%</div><div>••</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 29087 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 DNA chain called DNA (5'-D(\*GP\*CP\*AP\*GP\*TP\*CP\*AP\*TP\*CP\*AP\*CP\*CP\*AP\*AP\*TP\*TP\*TP\*AP\*TP\*TP\*TP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	7	Total	C	N	O	P	0	0
			140	67	26	40	7		

- Molecule 2 is a DNA chain called DNA (100-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	39	Total	C	N	O	P	0	0
			807	382	161	225	39		

- Molecule 3 is a RNA chain called RNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	61	Total	C	N	O	P	0	0
			1275	569	219	427	60		

- Molecule 4 is a protein called Cas8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	450	Total	C	N	O	S	0	0
			3538	2244	615	661	18		

- Molecule 5 is a protein called Cas7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	338	Total	C	N	O	S	0	0
			2704	1720	464	505	15		
5	C	339	Total	C	N	O	S	0	0
			2713	1726	466	506	15		
5	D	341	Total	C	N	O	S	0	0
			2729	1736	469	509	15		
5	F	341	Total	C	N	O	S	0	0
			2729	1736	469	509	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	340	Total	C	N	O	S	0	0
			2720	1730	467	508	15		
5	G	307	Total	C	N	O	S	0	0
			2490	1591	428	457	14		

- Molecule 6 is a protein called Cas6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	135	Total	C	N	O	S	0	0
			1113	712	203	192	6		

- Molecule 7 is a protein called TniQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	374	Total	C	N	O	S	0	0
			3050	1959	522	550	19		
7	J	378	Total	C	N	O	S	0	0
			3075	1975	526	555	19		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	J	2	Total	Zn	0
			2	2	
8	I	2	Total	Zn	0
			2	2	



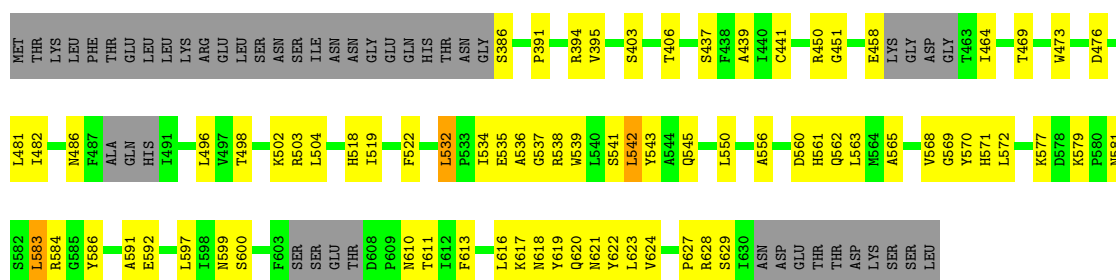
- Molecule 1: DNA (5'-D(\*GP\*CP\*AP\*GP\*TP\*CP\*AP\*TP\*CP\*AP\*CP\*CP\*AP\*AP\*TP\*TP\*TP\*AP\*TP\*TP\*TP\*A)-3')

DG	DC	DA	DG	DT	DC	DA	T8	C9	A10	C11	A14	DT	DT	DT	DA	DT	DT	DT	DA
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[illegible]

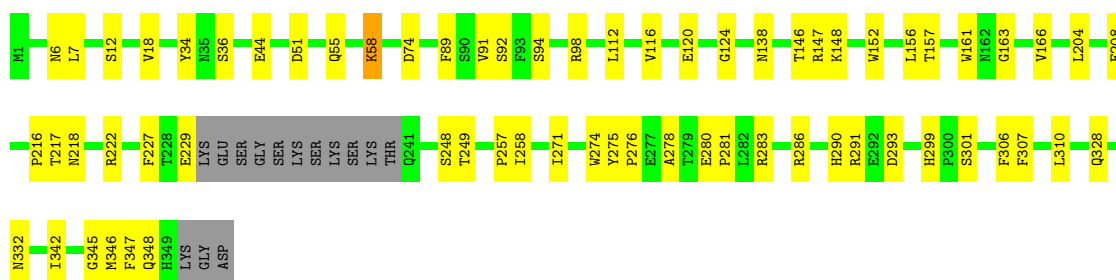
C1	U2	G3	A6	U9	U10	G14	G15	A16	G17	C18	C19	U20	U21	U22	U27	C28	G32	C33	U34	U35	U36	U37	C38	A39	G40	G41	U42	G43	A44	A45	C46	U47	G48	C49	G50	A51	A52	G53	U54	G60	A61	U58	A59	G60	A61
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[illegible]



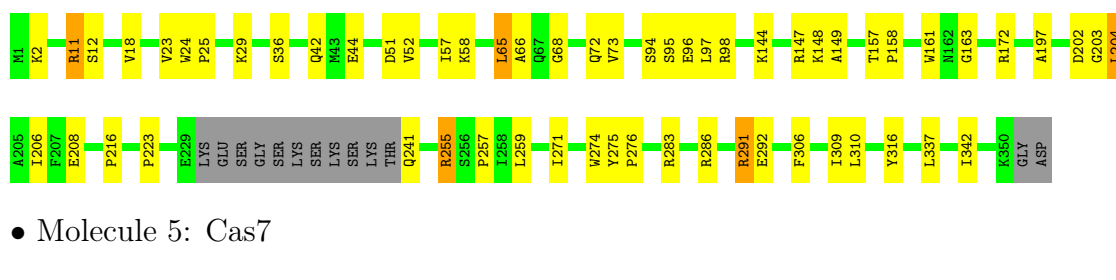
### • Molecule 5: Cas7

Chain B: 77% 18% .



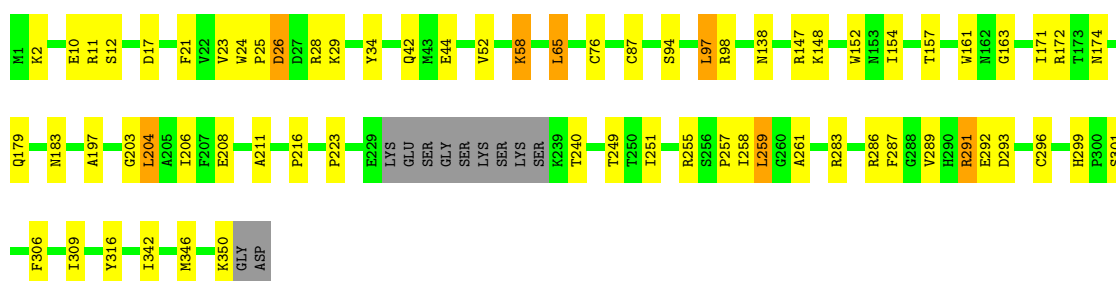
### • Molecule 5: Cas7

Chain C: 79% 16% . .



### • Molecule 5: Cas7

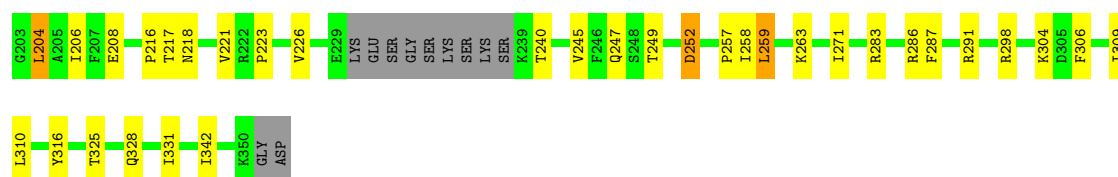
Chain D: 78% 17% . .



### • Molecule 5: Cas7

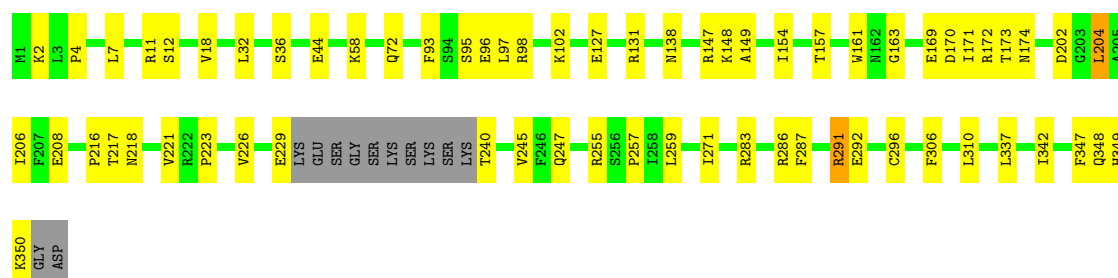
Chain F: 78% 18% . .





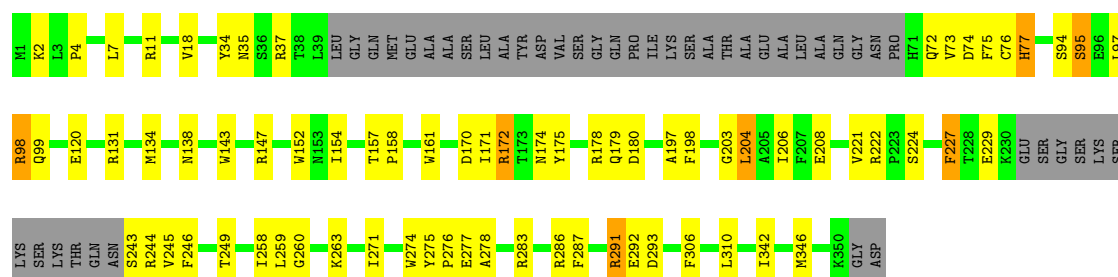
• Molecule 5: Cas7

Chain E: 78% 18% . .



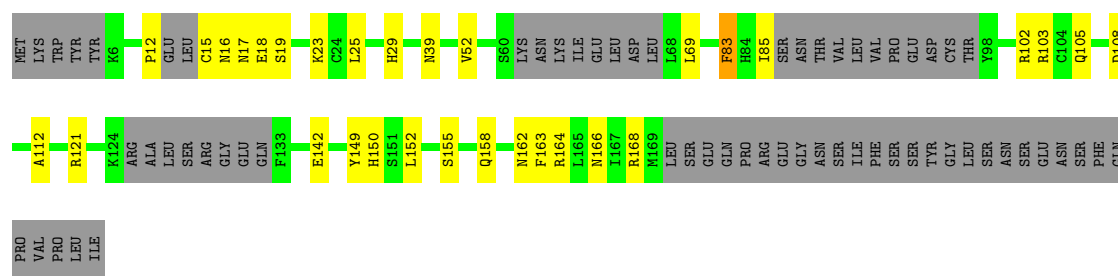
• Molecule 5: Cas7

Chain G: 66% 19% . 13%



• Molecule 6: Cas6

Chain H: 52% 15% . 32%

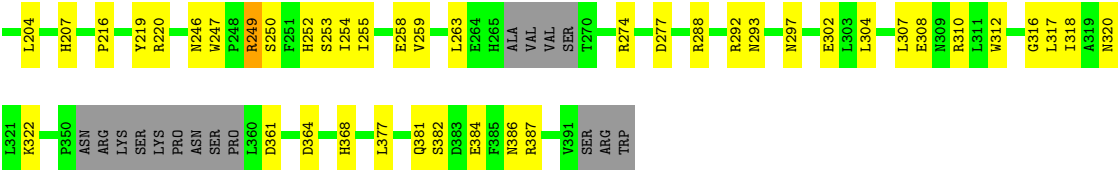


• Molecule 7: TniQ

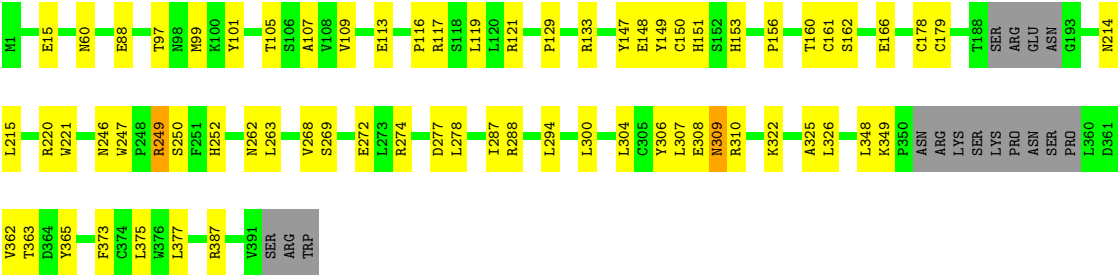
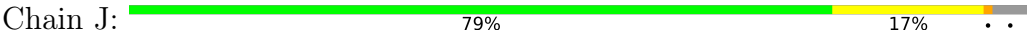
Chain I: 77% 18% 5%







• Molecule 7: ThiQ



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55900	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2.16	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K3 (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: ZN

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  >2	RMSZ	# Z  >2
1	M	0.74	0/156	0.84	0/237
2	L	1.27	0/909	0.91	0/1401
3	K	0.95	0/1423	1.05	0/2216
4	A	0.45	0/3611	0.65	0/4894
5	B	0.51	0/2775	0.65	0/3771
5	C	0.61	0/2784	0.70	0/3782
5	D	0.66	0/2800	0.73	0/3803
5	E	0.63	0/2791	0.72	0/3792
5	F	0.61	0/2800	0.71	0/3803
5	G	0.54	0/2557	0.68	0/3470
6	H	0.34	0/1135	0.57	0/1519
7	I	0.30	0/3134	0.51	0/4243
7	J	0.30	0/3160	0.48	0/4281
All	All	0.58	0/30035	0.69	0/41212

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	M	140	0	79	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	807	0	436	15	0
3	K	1275	0	642	60	0
4	A	3538	0	3528	158	0
5	B	2704	0	2632	60	0
5	C	2713	0	2645	48	0
5	D	2729	0	2665	64	0
5	E	2720	0	2652	56	0
5	F	2729	0	2665	46	0
5	G	2490	0	2433	111	0
6	H	1113	0	1113	52	0
7	I	3050	0	2960	53	0
7	J	3075	0	2992	58	0
8	I	2	0	0	0	0
8	J	2	0	0	0	0
All	All	29087	0	27442	653	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 12.

The worst 5 of 653 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)
4:A:560:ASP:CB	4:A:563:LEU:HD13	1.46	1.44
4:A:611:THR:HG22	4:A:629:SER:CB	1.52	1.39
4:A:619:TYR:HD2	4:A:622:TYR:CE2	1.46	1.30
6:H:12:PRO:CG	6:H:15:CYS:HB3	1.65	1.26
4:A:619:TYR:CD2	4:A:622:TYR:CE2	2.28	1.21

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	
4	A	432/640 (68%)	380 (88%)	50 (12%)	2 (0%)	31	71
5	B	334/352 (95%)	301 (90%)	33 (10%)	0	100	100
5	C	335/352 (95%)	304 (91%)	31 (9%)	0	100	100
5	D	337/352 (96%)	315 (94%)	22 (6%)	0	100	100
5	E	336/352 (96%)	305 (91%)	31 (9%)	0	100	100
5	F	337/352 (96%)	303 (90%)	34 (10%)	0	100	100
5	G	301/352 (86%)	274 (91%)	27 (9%)	0	100	100
6	H	125/199 (63%)	113 (90%)	12 (10%)	0	100	100
7	I	366/394 (93%)	344 (94%)	22 (6%)	0	100	100
7	J	372/394 (94%)	354 (95%)	17 (5%)	1 (0%)	43	79
All	All	3275/3739 (88%)	2993 (91%)	279 (8%)	3 (0%)	56	87

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	536	ALA
4	A	620	GLN
7	J	307	LEU

### 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	
4	A	400/573 (70%)	391 (98%)	9 (2%)	53	81
5	B	296/308 (96%)	291 (98%)	5 (2%)	63	86
5	C	297/308 (96%)	286 (96%)	11 (4%)	37	72
5	D	299/308 (97%)	285 (95%)	14 (5%)	29	66
5	E	298/308 (97%)	291 (98%)	7 (2%)	53	81
5	F	299/308 (97%)	289 (97%)	10 (3%)	41	74
5	G	275/308 (89%)	262 (95%)	13 (5%)	29	66
6	H	121/181 (67%)	118 (98%)	3 (2%)	50	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I	337/356 (95%)	336 (100%)	1 (0%)	93	97
7	J	340/356 (96%)	338 (99%)	2 (1%)	87	95
All	All	2962/3314 (89%)	2887 (98%)	75 (2%)	54	80

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	174	ASN
5	F	58	LYS
6	H	39	ASN
5	D	204	LEU
5	D	291	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
5	C	349	HIS
5	E	77	HIS
7	J	66	ASN
5	D	299	HIS
4	A	562	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	K	59/61 (96%)	35 (59%)	12 (20%)

5 of 35 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	K	3	G
3	K	6	A
3	K	9	U
3	K	10	U
3	K	14	G

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	K	34	U
3	K	36	U
3	K	42	U
3	K	21	U
3	K	41	G

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.