Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Sep 19, 2019 – 10:22 AM EDT

PDB ID	:	6QX3
EMDB ID:	:	EMD-4661
Title	:	Influenza A virus (A/NT/60/1968) polymerase Hetermotrimer in complex with 3'5' cRNA promoter and Nb8205
Authors	:	Carrique, L.; Keown, J.R.; Fan, H.; Fodor, E.; Grimes, J.M.
Deposited on	:	2019-03-07
Resolution	:	3.79 Å(reported)
Based on PDB ID	:	6QPG

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB 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 (i) symbol.

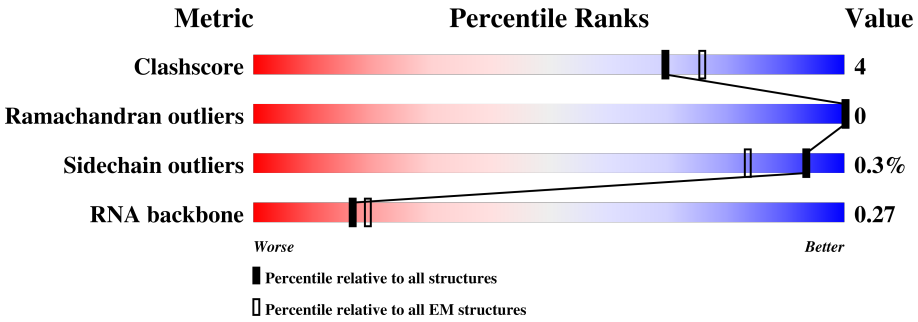
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.79 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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	D	15	33% 27% 7% 33%
2	G	15	7% 13% 7% 73%
3	O	134	83% 7% 10%
4	B	757	73% 9% 19%
5	A	716	64% 8% 28%
6	C	762	10% 89%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21587 atoms, of which 10646 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 RNA chain called RNA (5'-R(P*AP*GP*CP*AP*AP*AP*AP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	D	10	329	98	111	46	64	10	0	0

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*CP*U)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	G	4	122	36	42	9	31	4	0	0

- Molecule 3 is a protein called Nb8205.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	O	121	1799	572	877	163	181	6	0	0

- Molecule 4 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	B	615	9750	3084	4858	850	923	35	0	0

- Molecule 5 is a protein called Polymerase acidic protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	A	515	8157	2614	4039	691	783	30	0	0

- Molecule 6 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	C	86	1430	453	719	125	125	8	0	0

There are 6 discrepancies between the modelled and reference sequences:

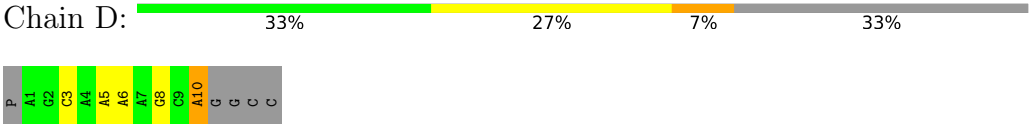
Chain	Residue	Modelled	Actual	Comment	Reference
C	757	GLU	-	expression tag	UNP P03429
C	758	ASN	-	expression tag	UNP P03429
C	759	LEU	-	expression tag	UNP P03429
C	760	TYR	-	expression tag	UNP P03429
C	761	PHE	-	expression tag	UNP P03429
C	762	GLN	-	expression tag	UNP P03429

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: RNA (5'-R(P*AP*GP*CP*AP*AP*AP*AP*GP*CP*A)-3')

Chain D:

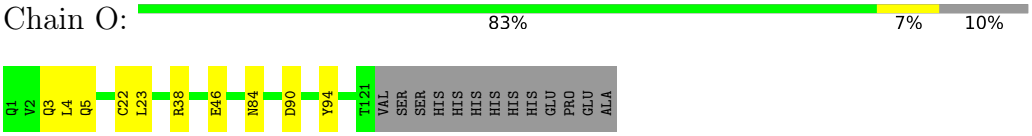


• Molecule 2: RNA (5'-R(P*UP*UP*CP*U)-3')

Chain G:

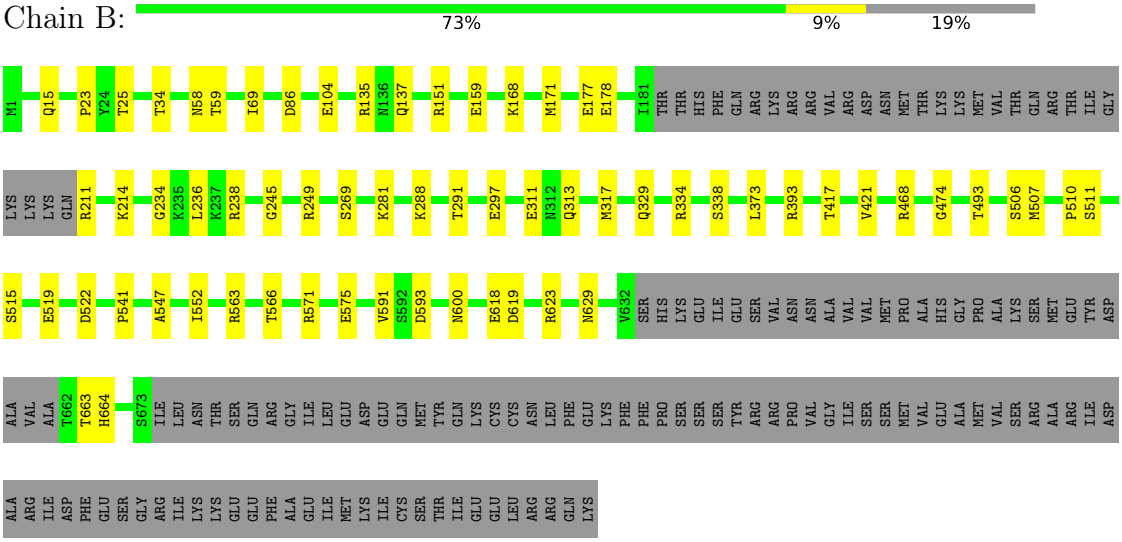
• Molecule 3: Nb8205

Chain O:



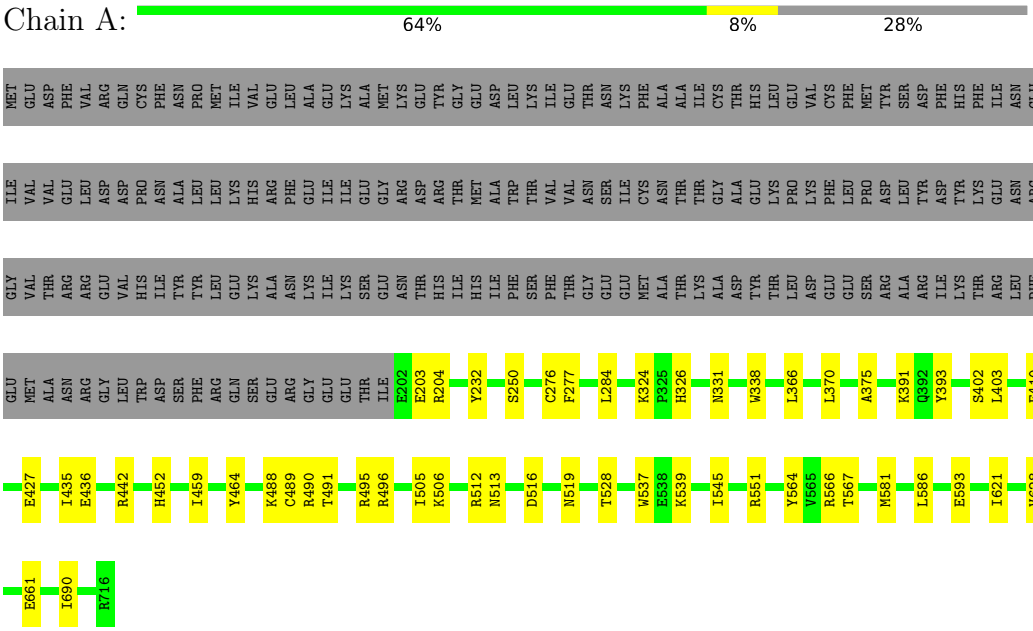
• Molecule 4: RNA-directed RNA polymerase catalytic subunit

Chain B:



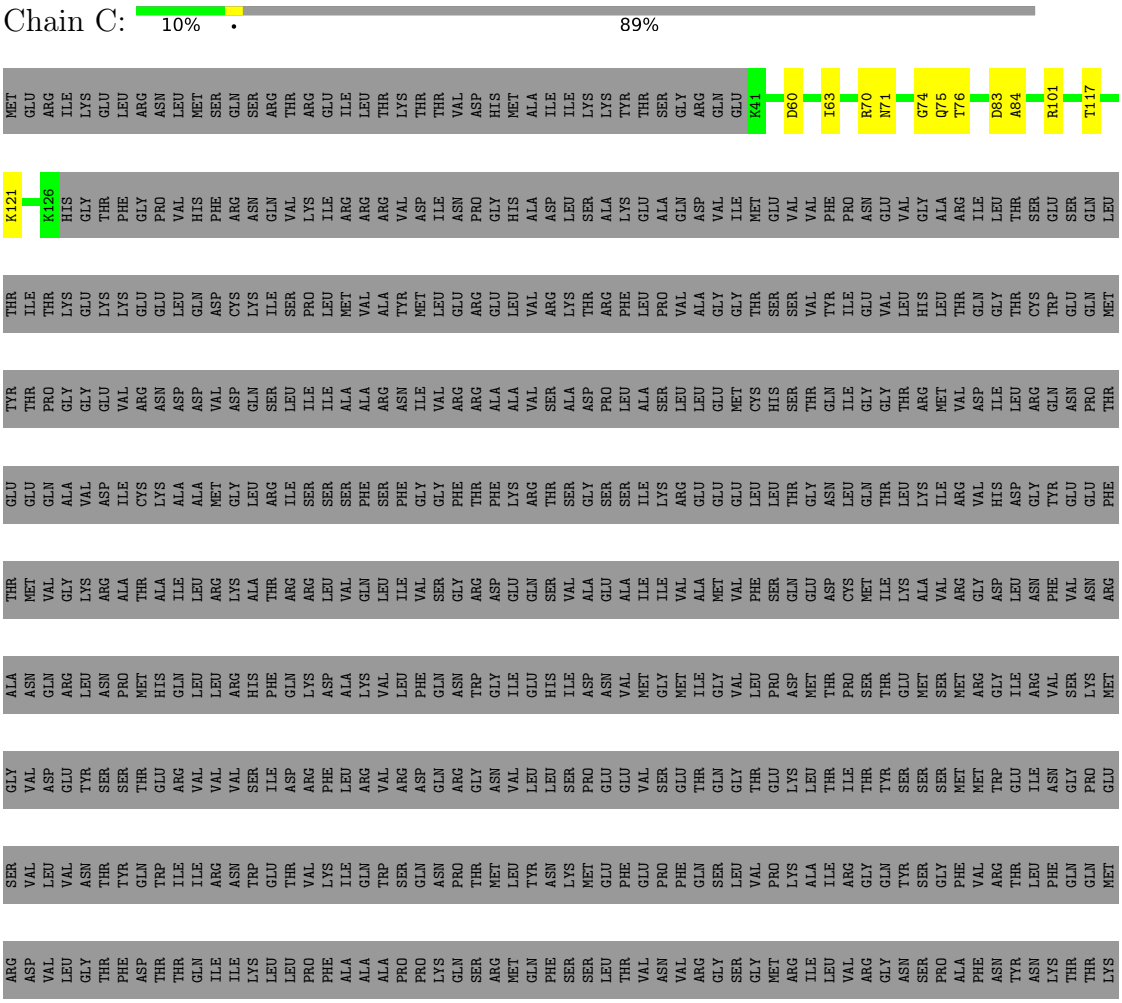
• Molecule 5: Polymerase acidic protein

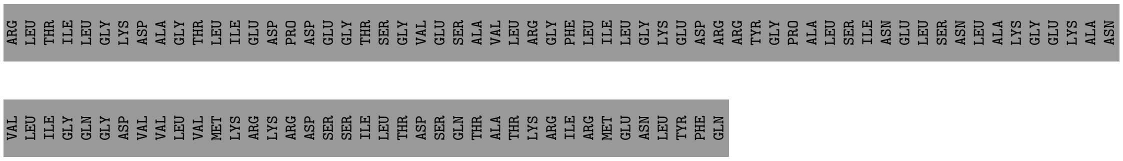
Chain A:



• Molecule 6: Polymerase basic protein 2

Chain C:




ARG LEU THR ILE LEU GLY LYS ASP ALA GLY THR LEU ILE GLU ASP PRO ASP GLU GLY THR SER GLY VAL GLU SER ALA VAL LEU ARG GLY PHE LEU ILE LEU GLY LYS GLU ASP ARG ARG TYR GLY PRO ALA LEU SER ILE ASN GLU LEU SER ASN LEU ALA LYS GLY GLU LYS ALA ASN
VAL LEU ILE GLY GLN GLY ASP VAL VAL LEU VAL MET LYS ARG LYS ARG ASP SER SER ILE LEU THR ASP SER GLN THR ALA THR LYS ARG ILE ARG MET GLU ASN LEU TYR PHE GLN

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52932	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 ($e^-/Å^2$)	1.25	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	D	0.29	0/245	0.72	0/380
2	G	0.36	0/87	1.68	5/132 (3.8%)
3	O	0.35	0/942	0.56	0/1278
4	B	0.33	0/4991	0.54	0/6744
5	A	0.37	0/4209	0.54	0/5688
6	C	0.27	0/730	0.51	0/985
All	All	0.34	0/11204	0.56	5/15207 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	11	C	C2-N1-C1'	9.14	128.85	118.80
2	G	11	C	N1-C2-O2	7.03	123.12	118.90
2	G	11	C	C6-N1-C1'	-6.33	113.20	120.80
2	G	11	C	N3-C2-O2	-6.18	117.57	121.90
2	G	11	C	C6-N1-C2	-5.93	117.93	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	D	218	111	111	3	0
2	G	80	42	42	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	922	877	877	7	0
4	B	4892	4858	4856	42	0
5	A	4118	4039	4037	39	0
6	C	711	719	719	7	0
All	All	10941	10646	10642	86	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 (86) 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:B:563:ARG:O	4:B:566:THR:OG1	2.05	0.74
5:A:566:ARG:NE	5:A:567:THR:O	2.22	0.72
3:O:90:ASP:OD1	3:O:94:TYR:OH	2.08	0.71
4:B:619:ASP:OD1	4:B:623:ARG:NH1	2.25	0.70
2:G:11:C:OP2	5:A:488:LYS:NZ	2.24	0.69
3:O:38:ARG:NH1	3:O:90:ASP:OD1	2.25	0.69
6:C:117:THR:O	6:C:121:LYS:NZ	2.23	0.69
5:A:513:ASN:ND2	5:A:516:ASP:OD1	2.26	0.68
4:B:629:ASN:ND2	4:B:663:THR:OG1	2.27	0.68
3:O:84:ASN:OD1	5:A:495:ARG:NH2	2.28	0.67
5:A:442:ARG:NH1	5:A:593:GLU:OE1	2.28	0.67
4:B:86:ASP:OD1	5:A:232:TYR:OH	2.12	0.66
4:B:334:ARG:O	4:B:338:SER:OG	2.14	0.65
4:B:23:PRO:HB2	4:B:25:THR:HG22	1.80	0.63
4:B:575:GLU:OE1	6:C:101:ARG:NE	2.30	0.63
4:B:104:GLU:OE1	4:B:329:GLN:NE2	2.32	0.62
5:A:370:LEU:O	5:A:519:ASN:ND2	2.32	0.61
4:B:151:ARG:NH2	4:B:159:GLU:OE1	2.32	0.61
3:O:22:CYS:SG	3:O:23:LEU:N	2.74	0.61
4:B:178:GLU:OE2	4:B:211:ARG:N	2.35	0.60
3:O:46:GLU:N	3:O:46:GLU:OE1	2.34	0.59
5:A:489:CYS:SG	5:A:490:ARG:N	2.76	0.59
6:C:70:ARG:NH1	6:C:76:THR:OG1	2.37	0.58
6:C:71:ASN:OD1	6:C:75:GLN:N	2.36	0.58
4:B:373:LEU:O	4:B:393:ARG:NH1	2.37	0.57
4:B:135:ARG:O	4:B:137:GLN:NE2	2.38	0.56
1:D:8:G:OP1	4:B:34:THR:OG1	2.18	0.56
4:B:171:MET:SD	5:A:204:ARG:NH2	2.79	0.56
4:B:515:SER:OG	4:B:522:ASP:OD1	2.10	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:311:GLU:N	4:B:311:GLU:OE1	2.40	0.55
4:B:552:ILE:HD11	4:B:591:VAL:HG11	1.87	0.55
4:B:168:LYS:NZ	5:A:203:GLU:O	2.38	0.54
5:A:326:HIS:N	5:A:331:ASN:OD1	2.41	0.54
4:B:245:GLY:O	4:B:249:ARG:NH1	2.41	0.53
4:B:15:GLN:N	4:B:15:GLN:OE1	2.42	0.53
1:D:3:C:OP2	5:A:539:LYS:NZ	2.40	0.53
4:B:297:GLU:N	4:B:297:GLU:OE1	2.42	0.53
4:B:69:ILE:HD12	4:B:317:MET:SD	2.50	0.52
6:C:83:ASP:OD1	6:C:84:ALA:N	2.40	0.52
5:A:661:GLU:O	5:A:690:ILE:HD11	2.09	0.52
4:B:236:LEU:O	4:B:238:ARG:NH2	2.42	0.52
4:B:618:GLU:N	4:B:618:GLU:OE1	2.43	0.51
5:A:417:LEU:HD23	5:A:452:HIS:O	2.10	0.51
5:A:324:LYS:NZ	5:A:537:TRP:O	2.40	0.50
5:A:491:THR:HG22	5:A:495:ARG:O	2.12	0.50
4:B:468:ARG:NH2	5:A:250:SER:O	2.45	0.50
4:B:600:ASN:ND2	5:A:436:GLU:OE2	2.43	0.49
5:A:366:LEU:CD1	5:A:505:ILE:HG21	2.44	0.48
4:B:234:GLY:N	5:A:656:GLU:OE2	2.46	0.48
4:B:58:ASN:OD1	4:B:59:THR:N	2.47	0.48
6:C:70:ARG:NH1	6:C:74:GLY:O	2.45	0.47
4:B:519:GLU:OE1	4:B:664:HIS:ND1	2.44	0.47
5:A:459:ILE:HG23	5:A:581:MET:HB3	1.96	0.47
5:A:276:CYS:SG	5:A:277:PHE:N	2.88	0.47
2:G:9:U:OP1	4:B:571:ARG:NH2	2.48	0.46
4:B:510:PRO:O	4:B:511:SER:OG	2.29	0.46
5:A:528:THR:O	5:A:564:TYR:OH	2.34	0.46
5:A:427:GLU:OE2	5:A:427:GLU:N	2.45	0.46
1:D:10:A:H2'	5:A:375:ALA:HB2	1.98	0.45
4:B:541:PRO:CG	5:A:435:ILE:HD11	2.46	0.45
5:A:366:LEU:HD11	5:A:505:ILE:HG21	1.98	0.45
2:G:12:U:OP1	5:A:464:TYR:OH	2.35	0.45
4:B:269:SER:O	4:B:281:LYS:NZ	2.43	0.45
4:B:506:SER:OG	4:B:507:MET:N	2.49	0.45
2:G:11:C:O2'	2:G:12:U:OP1	2.35	0.44
4:B:547:ALA:HB2	5:A:586:LEU:HD11	2.00	0.44
4:B:313:GLN:NE2	4:B:474:GLY:O	2.51	0.44
5:A:628:VAL:HG23	5:A:628:VAL:O	2.18	0.44
5:A:402:SER:OG	5:A:403:LEU:N	2.50	0.43
5:A:424:GLU:OE2	5:A:490:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:177:GLU:O	4:B:214:LYS:N	2.51	0.43
4:B:288:LYS:O	4:B:291:THR:HG22	2.19	0.43
5:A:338:TRP:HE1	5:A:545:ILE:HD12	1.84	0.42
4:B:593:ASP:OD1	4:B:593:ASP:N	2.52	0.42
4:B:493:THR:O	4:B:493:THR:HG22	2.20	0.42
3:O:3:GLN:C	3:O:4:LEU:HD12	2.40	0.42
5:A:284:LEU:HD12	5:A:410:GLU:OE2	2.20	0.42
4:B:541:PRO:HG2	5:A:435:ILE:HD11	2.02	0.41
6:C:60:ASP:O	6:C:63:ILE:HG22	2.21	0.41
5:A:621:ILE:HG21	5:A:636:VAL:HG22	2.02	0.41
3:O:5:GLN:N	3:O:5:GLN:OE1	2.53	0.41
5:A:512:ARG:N	5:A:516:ASP:OD2	2.53	0.41
2:G:9:U:O2'	2:G:10:U:OP1	2.35	0.41
5:A:391:LYS:NZ	5:A:393:TYR:O	2.54	0.40
4:B:417:THR:O	4:B:421:VAL:HG23	2.21	0.40
2:G:12:U:O2'	5:A:424:GLU:OE1	2.26	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	
3	O	119/134 (89%)	108 (91%)	11 (9%)	0	100	100
4	B	609/757 (80%)	549 (90%)	60 (10%)	0	100	100
5	A	513/716 (72%)	463 (90%)	50 (10%)	0	100	100
6	C	84/762 (11%)	77 (92%)	7 (8%)	0	100	100
All	All	1325/2369 (56%)	1197 (90%)	128 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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
3	O	97/111 (87%)	97 (100%)	0	100 100
4	B	538/669 (80%)	538 (100%)	0	100 100
5	A	453/644 (70%)	450 (99%)	3 (1%)	85 93
6	C	79/674 (12%)	79 (100%)	0	100 100
All	All	1167/2098 (56%)	1164 (100%)	3 (0%)	93 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	496	ARG
5	A	506	LYS
5	A	551	ARG

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

Mol	Chain	Res	Type
4	B	629	ASN
5	A	587	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	9/15 (60%)	3 (33%)	0
2	G	3/15 (20%)	3 (100%)	0
All	All	12/30 (40%)	6 (50%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	5	A
1	D	6	A

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Mol	Chain	Res	Type
1	D	10	A
2	G	10	U
2	G	11	C
2	G	12	U

There are no RNA pucker outliers to report.

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)

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)

There are no chain breaks in this entry.