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

Dec 22, 2018 – 11:07 PM EST

PDB ID	:	6G1X
EMDB ID:	:	EMD-4341
Title	:	CryoEM structure of the MDA5-dsRNA filament with 91-degree helical twist
Authors	:	Yu, Q.; Qu, K.; Modis, Y.
Deposited on	:	2018-03-22
Resolution	:	3.93 Å(reported)

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.

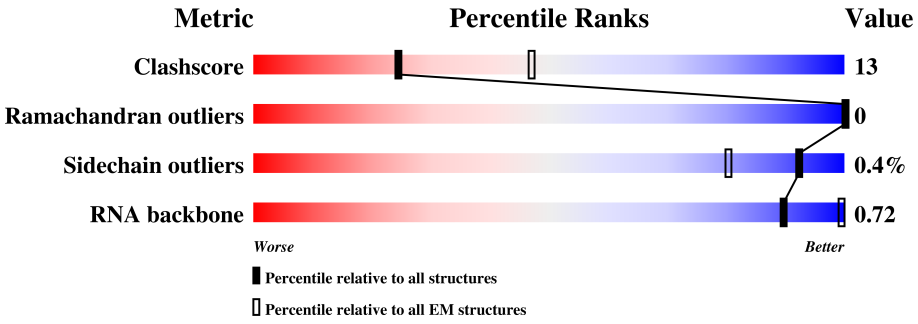
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

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 3.93 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	A	696	71% 22% • 7%
2	X	15	93% 7%
3	Y	15	100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9989 atoms, of which 4182 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 Interferon-induced helicase C domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	648	9349	3287	4182	896	949	35	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q8R5F7
A	?	-	LYS	deletion	UNP Q8R5F7
A	?	-	SER	deletion	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7
A	?	-	GLU	deletion	UNP Q8R5F7
A	?	-	ALA	deletion	UNP Q8R5F7
A	?	-	SER	deletion	UNP Q8R5F7
A	?	-	SER	deletion	UNP Q8R5F7
A	?	-	CYS	deletion	UNP Q8R5F7
A	?	-	ASN	deletion	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7
A	?	-	GLN	deletion	UNP Q8R5F7
A	?	-	LEU	deletion	UNP Q8R5F7
A	?	-	LYS	deletion	UNP Q8R5F7
A	?	-	GLY	deletion	UNP Q8R5F7
A	?	-	ASP	deletion	UNP Q8R5F7
A	?	-	VAL	deletion	UNP Q8R5F7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	X	15	318	142	56	105	15	0	0

- Molecule 3 is a RNA chain called RNA (5'-R(P*CP*GP*UP*CP*AP*UP*GP*CP*GP*CP

*AP*UP*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Y	15	Total	C	N	O	P	0	0
			321	143	58	105	15		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

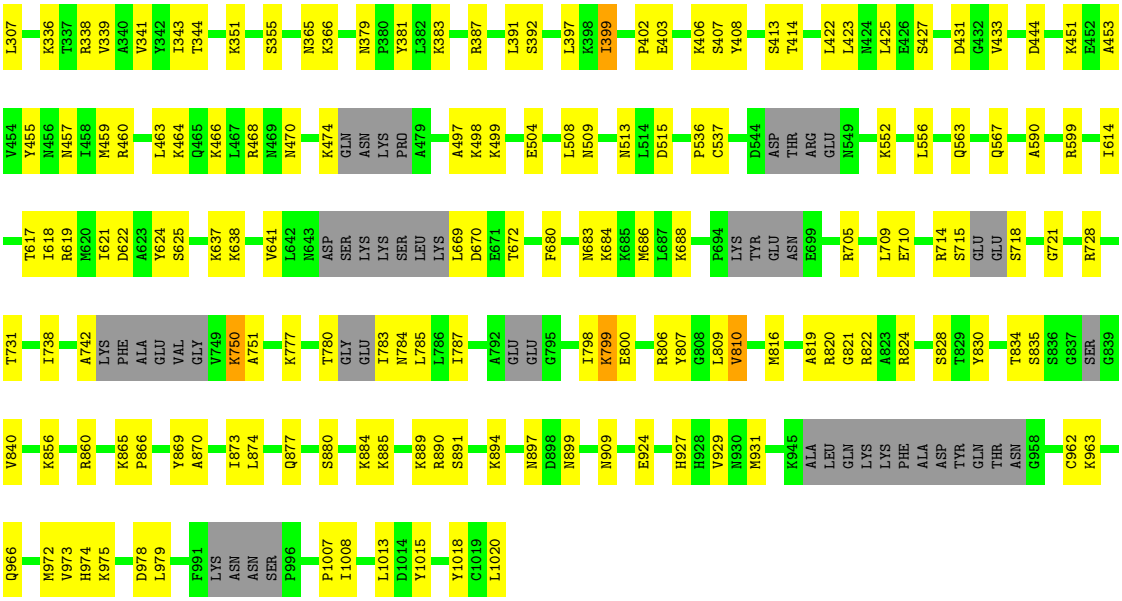
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	

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.

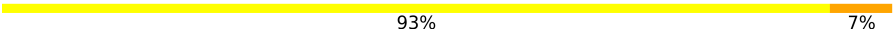
• Molecule 1: Interferon-induced helicase C domain-containing protein 1

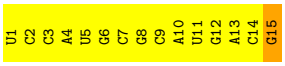
Chain A:



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

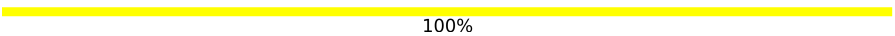
Chain X:

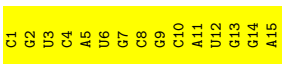




• Molecule 3: RNA (5'-R(P*CP*GP*UP*CP*AP*UP*GP*CP*GP*CP*AP*UP*GP*GP*A)-3')

Chain Y:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=90.9214°, rise=44.9703 Å, axial sym=C1	Depositor
Number of segments used	39987	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 ($e^-/Å^2$)	29.85	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	A	0.55	0/5242	0.62	2/7039 (0.0%)
2	X	0.95	0/354	0.99	0/549
3	Y	0.94	0/358	0.88	0/556
All	All	0.61	0/5954	0.67	2/8144 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	497	ALA	C-N-CA	6.12	137.00	121.70
1	A	399	ILE	C-N-CA	5.75	136.06	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	810	VAL	Peptide

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	5167	4182	5287	107	0
2	X	318	0	163	23	0
3	Y	321	0	163	22	0
4	A	1	0	0	0	0
All	All	5807	4182	5613	146	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 13.

All (146) 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)
2:X:3:C:H2'	2:X:4:A:H8	1.42	0.83
1:A:444:ASP:O	1:A:455:TYR:OH	2.01	0.78
1:A:599:ARG:NH1	1:A:909:ASN:OD1	2.18	0.77
1:A:777:LYS:O	1:A:780:THR:OG1	2.05	0.74
1:A:909:ASN:ND2	1:A:966:GLN:OE1	2.20	0.73
1:A:974:HIS:HB3	1:A:975:LYS:HD2	1.71	0.73
1:A:821:GLY:O	1:A:824:ARG:NE	2.17	0.72
1:A:351:LYS:O	1:A:355:SER:N	2.22	0.72
2:X:9:C:H2'	2:X:10:A:H8	1.54	0.71
1:A:423:LEU:O	1:A:427:SER:N	2.20	0.70
2:X:9:C:H2'	2:X:10:A:C8	2.27	0.69
1:A:715:SER:O	1:A:718:SER:N	2.24	0.69
2:X:5:U:H2'	2:X:6:G:H8	1.57	0.69
1:A:341:VAL:O	1:A:344:THR:OG1	2.11	0.68
3:Y:1:C:H2'	3:Y:2:G:H8	1.58	0.67
1:A:751:ALA:HB2	1:A:785:LEU:HD21	1.76	0.67
1:A:810:VAL:HG21	2:X:13:A:H5'	1.77	0.67
2:X:3:C:H2'	2:X:4:A:C8	2.29	0.67
1:A:824:ARG:O	1:A:828:SER:OG	2.14	0.66
3:Y:1:C:H2'	3:Y:2:G:C8	2.30	0.66
1:A:891:SER:HA	1:A:894:LYS:HG2	1.76	0.66
3:Y:3:U:H2'	3:Y:4:C:H6	1.61	0.65
2:X:5:U:H2'	2:X:6:G:C8	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:4:C:H2'	3:Y:5:A:C8	2.31	0.65
1:A:336:LYS:NZ	1:A:444:ASP:OD1	2.30	0.64
3:Y:8:C:H2'	3:Y:9:G:H8	1.62	0.64
3:Y:4:C:H2'	3:Y:5:A:H8	1.63	0.64
1:A:927:HIS:NE2	2:X:5:U:O2'	2.28	0.63
1:A:614:ILE:O	1:A:618:ILE:N	2.30	0.63
1:A:617:THR:O	1:A:807:TYR:OH	2.16	0.63
1:A:806:ARG:HD2	1:A:809:LEU:CD2	2.29	0.62
1:A:897:ASN:HB2	1:A:1007:PRO:HG2	1.80	0.62
1:A:453:ALA:HB2	2:X:10:A:H5'	1.81	0.62
3:Y:10:C:O2'	3:Y:11:A:H5'	2.00	0.62
1:A:379:ASN:O	1:A:383:LYS:N	2.32	0.62
1:A:464:LYS:HE2	1:A:468:ARG:HH21	1.66	0.61
1:A:834:THR:HG21	1:A:840:VAL:HG21	1.82	0.61
1:A:865:LYS:HD2	1:A:866:PRO:HD2	1.83	0.61
1:A:425:LEU:HB2	1:A:433:VAL:H	1.66	0.60
1:A:339:VAL:O	1:A:343:ILE:HD12	2.00	0.60
3:Y:8:C:H2'	3:Y:9:G:C8	2.37	0.60
1:A:806:ARG:HD2	1:A:809:LEU:HD23	1.83	0.59
3:Y:3:U:H2'	3:Y:4:C:C6	2.38	0.59
1:A:590:ALA:HB3	1:A:599:ARG:HB3	1.85	0.59
1:A:619:ARG:HG3	1:A:621:ILE:HG22	1.85	0.59
2:X:8:G:O2'	2:X:9:C:H5'	2.03	0.58
2:X:7:C:H2'	2:X:8:G:H8	1.68	0.58
2:X:12:G:H2'	2:X:13:A:H8	1.70	0.57
1:A:451:LYS:HD2	1:A:880:SER:HA	1.87	0.57
1:A:683:ASN:O	1:A:686:MET:HG2	2.05	0.56
1:A:307:LEU:HB3	1:A:381:TYR:CD2	2.40	0.56
1:A:402:PRO:HG2	1:A:431:ASP:HB3	1.88	0.56
3:Y:7:G:O2'	3:Y:8:C:H5'	2.06	0.56
2:X:7:C:H2'	2:X:8:G:C8	2.40	0.55
2:X:12:G:H2'	2:X:13:A:C8	2.42	0.55
1:A:798:ILE:HB	1:A:822:ARG:HD2	1.87	0.55
1:A:890:ARG:O	1:A:894:LYS:HG2	2.07	0.55
1:A:459:MET:O	1:A:463:LEU:HG	2.07	0.55
1:A:1018:TYR:O	1:A:1020:LEU:HD12	2.07	0.55
1:A:891:SER:HA	1:A:894:LYS:CG	2.37	0.55
1:A:710:GLU:O	1:A:714:ARG:HG3	2.06	0.55
1:A:413:SER:OG	1:A:414:THR:N	2.40	0.54
2:X:4:A:O2'	2:X:5:U:H5'	2.07	0.54
1:A:536:PRO:HB2	1:A:828:SER:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ASP:OD1	1:A:877:GLN:NE2	2.40	0.54
1:A:622:ASP:O	1:A:625:SER:OG	2.21	0.53
3:Y:14:G:H2'	3:Y:15:A:H8	1.71	0.53
1:A:962:CYS:HB3	1:A:966:GLN:N	2.23	0.53
1:A:728:ARG:NH2	3:Y:7:G:OP2	2.41	0.53
1:A:975:LYS:HG2	1:A:1015:TYR:OH	2.08	0.53
1:A:509:ASN:O	1:A:513:ASN:ND2	2.42	0.53
1:A:624:TYR:CE2	1:A:688:LYS:HD2	2.44	0.53
1:A:806:ARG:HG3	1:A:830:TYR:OH	2.09	0.53
1:A:399:ILE:HD11	1:A:403:GLU:HG3	1.91	0.52
3:Y:3:U:O2'	3:Y:4:C:H5'	2.10	0.52
1:A:552:LYS:HG2	1:A:556:LEU:CD1	2.40	0.52
1:A:391:LEU:O	1:A:392:SER:OG	2.25	0.51
1:A:731:THR:HG22	1:A:787:ILE:HG22	1.91	0.51
2:X:6:G:O2'	2:X:7:C:H5'	2.10	0.51
1:A:637:LYS:O	1:A:641:VAL:HG23	2.11	0.51
1:A:422:LEU:O	1:A:425:LEU:HB3	2.11	0.51
1:A:738:ILE:HG23	1:A:742:ALA:HB3	1.93	0.50
1:A:924:GLU:OE1	3:Y:12:U:O2'	2.22	0.50
3:Y:14:G:H2'	3:Y:15:A:C8	2.47	0.50
1:A:929:VAL:HG21	1:A:979:LEU:HB3	1.93	0.50
1:A:563:GLN:O	1:A:567:GLN:N	2.44	0.50
1:A:870:ALA:O	1:A:874:LEU:HG	2.12	0.49
1:A:962:CYS:SG	1:A:963:LYS:N	2.85	0.49
2:X:1:U:H2'	2:X:2:C:H6	1.77	0.49
3:Y:6:U:H2'	3:Y:7:G:C8	2.48	0.49
1:A:721:GLY:N	1:A:784:ASN:O	2.46	0.48
3:Y:14:G:O2'	3:Y:15:A:H5'	2.13	0.48
3:Y:2:G:O2'	3:Y:3:U:H5'	2.14	0.48
3:Y:6:U:H2'	3:Y:7:G:H8	1.78	0.48
1:A:464:LYS:HE2	1:A:468:ARG:NH2	2.29	0.48
1:A:466:LYS:NZ	1:A:515:ASP:OD2	2.35	0.47
1:A:619:ARG:CG	1:A:621:ILE:HG22	2.45	0.47
1:A:624:TYR:CZ	1:A:688:LYS:HD2	2.50	0.47
3:Y:13:G:O2'	3:Y:14:G:H5'	2.14	0.47
1:A:457:ASN:OD1	1:A:460:ARG:NH2	2.48	0.47
1:A:670:ASP:CG	1:A:672:THR:HG1	2.16	0.47
1:A:810:VAL:HG21	2:X:12:G:O2'	2.15	0.47
2:X:3:C:O2'	2:X:4:A:H5'	2.15	0.47
1:A:972:MET:HG2	1:A:974:HIS:HD2	1.81	0.46
2:X:1:U:H2'	2:X:2:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ASN:O	1:A:474:LYS:N	2.44	0.46
2:X:11:U:H2'	2:X:12:G:C8	2.50	0.46
1:A:504:GLU:O	1:A:508:LEU:HD23	2.16	0.46
3:Y:9:G:H2'	3:Y:10:C:H6	1.79	0.46
1:A:387:ARG:NH1	1:A:407:SER:OG	2.48	0.46
1:A:799:LYS:HD2	1:A:800:GLU:HB2	1.97	0.46
1:A:537:CYS:O	1:A:820:ARG:NH2	2.49	0.45
2:X:14:C:H2'	2:X:15:G:C8	2.50	0.45
1:A:705:ARG:HG2	1:A:709:LEU:HD12	1.97	0.45
3:Y:5:A:O2'	3:Y:6:U:H5'	2.15	0.45
1:A:391:LEU:HD13	1:A:397:LEU:HD22	1.99	0.45
1:A:365:ASN:OD1	1:A:366:LYS:N	2.50	0.45
1:A:816:MET:O	1:A:820:ARG:HG2	2.17	0.45
1:A:973:VAL:HG22	1:A:978:ASP:OD1	2.17	0.45
1:A:425:LEU:HD22	1:A:433:VAL:O	2.17	0.44
1:A:777:LYS:CB	1:A:783:ILE:HD12	2.48	0.44
1:A:899:ASN:H	1:A:1008:ILE:HA	1.81	0.44
1:A:806:ARG:HD2	1:A:809:LEU:HD22	1.99	0.44
1:A:931:MET:CE	1:A:1013:LEU:HD11	2.48	0.44
1:A:728:ARG:O	1:A:731:THR:OG1	2.21	0.43
1:A:856:LYS:O	1:A:860:ARG:HG3	2.19	0.43
1:A:869:TYR:O	1:A:873:ILE:HG12	2.19	0.43
1:A:403:GLU:O	1:A:407:SER:N	2.52	0.42
1:A:806:ARG:HH21	1:A:819:ALA:CB	2.32	0.42
1:A:638:LYS:HE2	1:A:669:LEU:HD23	2.01	0.42
1:A:750:LYS:HD2	1:A:750:LYS:H	1.85	0.42
1:A:806:ARG:HH22	1:A:816:MET:HA	1.84	0.42
2:X:10:A:O2'	2:X:11:U:H5'	2.19	0.42
1:A:407:SER:OG	1:A:408:TYR:N	2.53	0.42
1:A:498:LYS:HG3	1:A:499:LYS:HG3	2.02	0.42
1:A:338:ARG:HD2	1:A:381:TYR:HE2	1.85	0.41
1:A:899:ASN:HB2	1:A:1008:ILE:CG2	2.50	0.41
1:A:873:ILE:O	1:A:877:GLN:HG3	2.19	0.41
1:A:460:ARG:HE	1:A:884:LYS:HD2	1.84	0.41
1:A:834:THR:HG22	1:A:835:SER:O	2.21	0.41
1:A:785:LEU:HD23	1:A:785:LEU:H	1.85	0.41
1:A:402:PRO:O	1:A:406:LYS:HG3	2.21	0.40
1:A:751:ALA:CB	1:A:785:LEU:HD21	2.46	0.40
1:A:777:LYS:HB3	1:A:783:ILE:HD12	2.03	0.40
1:A:885:LYS:O	1:A:889:LYS:HG2	2.21	0.40
1:A:680:PHE:HE2	1:A:684:LYS:HD3	1.87	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	624/696 (90%)	545 (87%)	79 (13%)	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
1	A	571/625 (91%)	569 (100%)	2 (0%)	92 96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	750	LYS
1	A	799	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	ASN
1	A	513	ASN
1	A	711	GLN

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Mol	Chain	Res	Type
1	A	859	ASN
1	A	974	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	14/15 (93%)	1 (7%)	0
3	Y	14/15 (93%)	0	0
All	All	28/30 (93%)	1 (3%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	15	G

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)

Of 1 ligands modelled in this entry, 1 is 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.