

Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Feb 20, 2018 – 09:14 am GMT

PDB ID : 5Y36
EMDB ID: : EMD-8236
Title : Cryo-EM structure of SpCas9-sgRNA-DNA ternary complex
Authors : Huang, Q.; Li, G.; Huai, C.
Deposited on : 2017-07-27
Resolution : 5.20 Å(reported)
Based on PDB ID : 4OO8

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 ⓘ 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) : trunk30686

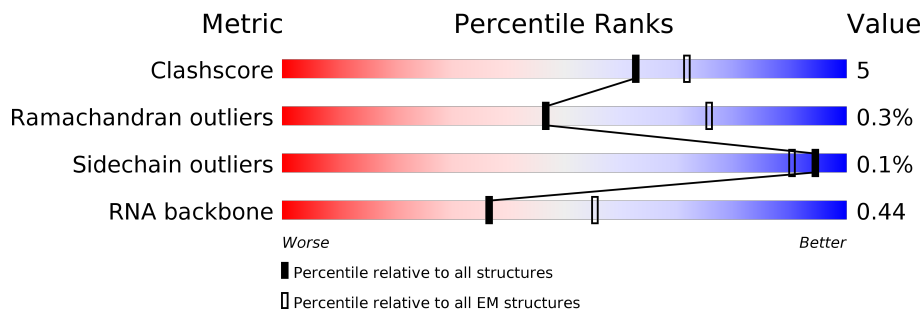
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.20 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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531
RNA backbone	3744	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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1368	
2	B	99	
3	C	41	
4	D	41	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14960 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 CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1368	11172	7109	1940	2099	24	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	ALA	ASP	engineered mutation	UNP Q99ZW2
A	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 2 is a RNA chain called single-guide RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	99	2110	945	379	688	98	0	0

- Molecule 3 is a DNA chain called complementary DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	41	843	402	156	245	40	0	0

- Molecule 4 is a DNA chain called non-complementary DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	41	832	398	151	243	40	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	A	2	Total	Mg	0
			2	2	

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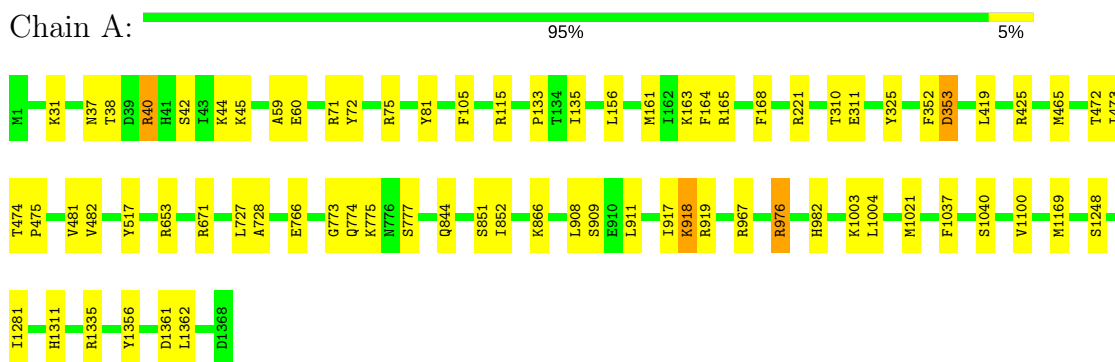
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	D	1	1	1	0

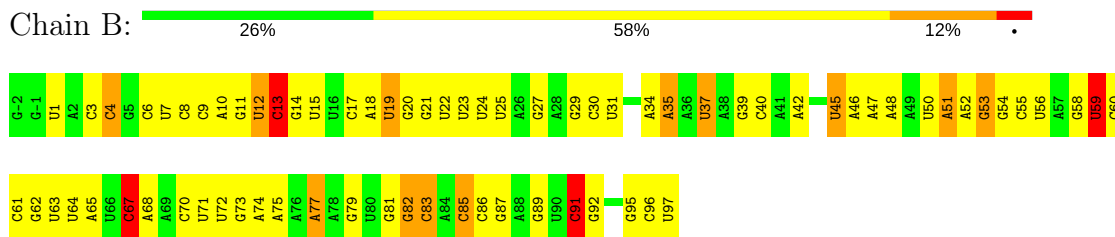
3 Residue-property plots

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.

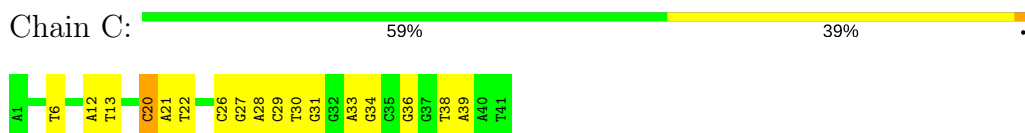
- Molecule 1: CRISPR-associated endonuclease Cas9/Csn1



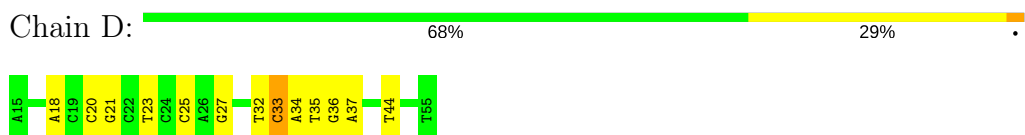
- Molecule 2: single-guide RNA



- Molecule 3: complementary DNA strand



- Molecule 4: non-complementary DNA strand



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57484	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	18000	Depositor
Image detector	GATAN K2 SUMMIT (4k 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: MG

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	0.73	0/11369	0.80	10/15275 (0.1%)
2	B	1.10	0/2361	1.40	58/3678 (1.6%)
3	C	1.28	0/946	1.45	20/1460 (1.4%)
4	D	1.25	0/932	1.25	8/1435 (0.6%)
All	All	0.88	0/15608	1.01	96/21848 (0.4%)

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	2

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	967	ARG	NE-CZ-NH1	14.42	127.51	120.30
3	C	30	DT	P-O3'-C3'	12.02	134.12	119.70
3	C	39	DA	P-O3'-C3'	11.52	133.53	119.70
3	C	12	DA	P-O3'-C3'	11.33	133.30	119.70
4	D	27	DG	P-O3'-C3'	10.25	132.00	119.70
3	C	13	DT	O4'-C4'-C3'	-10.23	99.86	106.00
4	D	27	DG	O4'-C4'-C3'	-10.20	99.88	106.00
3	C	6	DT	O4'-C4'-C3'	-9.36	100.39	106.00
4	D	44	DT	O4'-C4'-C3'	-9.31	100.41	106.00
4	D	25	DC	P-O3'-C3'	9.07	130.58	119.70
3	C	38	DT	O4'-C4'-C3'	-9.03	100.58	106.00
3	C	31	DG	O4'-C4'-C3'	-8.92	100.65	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	33	DC	P-O3'-C3'	8.90	130.38	119.70
3	C	28	DA	O4'-C4'-C3'	-8.83	100.70	106.00
3	C	31	DG	P-O3'-C3'	8.65	130.08	119.70
1	A	40	ARG	NE-CZ-NH1	8.58	124.59	120.30
2	B	27	G	O4'-C1'-N9	8.09	114.67	108.20
2	B	12	U	P-O3'-C3'	7.67	128.90	119.70
2	B	51	A	O4'-C1'-N9	7.64	114.31	108.20
2	B	9	C	O4'-C1'-N1	7.40	114.12	108.20
2	B	83	C	O4'-C1'-N1	7.29	114.03	108.20
3	C	27	DG	O4'-C4'-C3'	-7.26	101.59	104.50
2	B	91	C	O4'-C1'-N1	7.20	113.96	108.20
2	B	13	C	O4'-C1'-N1	7.15	113.92	108.20
2	B	61	C	O4'-C1'-N1	7.08	113.86	108.20
2	B	30	C	O4'-C1'-N1	7.01	113.81	108.20
2	B	6	C	O4'-C1'-N1	6.99	113.80	108.20
1	A	517	TYR	CB-CG-CD2	-6.99	116.81	121.00
2	B	8	C	O4'-C1'-N1	6.98	113.79	108.20
2	B	65	A	O4'-C1'-N9	6.98	113.79	108.20
2	B	40	C	O4'-C1'-N1	6.95	113.76	108.20
2	B	96	C	O4'-C1'-N1	6.84	113.67	108.20
2	B	70	C	O4'-C1'-N1	6.80	113.64	108.20
2	B	82	G	O4'-C1'-N9	6.74	113.59	108.20
1	A	967	ARG	NE-CZ-NH2	-6.69	116.96	120.30
2	B	60	C	O4'-C1'-N1	6.58	113.47	108.20
2	B	4	C	O4'-C1'-N1	6.52	113.42	108.20
2	B	45	U	O4'-C1'-N1	6.51	113.41	108.20
2	B	86	C	O4'-C1'-N1	6.39	113.31	108.20
2	B	17	C	O4'-C1'-N1	6.39	113.31	108.20
4	D	37	DA	O4'-C4'-C3'	-6.38	101.95	104.50
3	C	36	DG	P-O3'-C3'	6.37	127.34	119.70
2	B	67	C	O4'-C1'-N1	6.36	113.29	108.20
4	D	27	DG	C1'-O4'-C4'	-6.34	103.76	110.10
1	A	517	TYR	CB-CG-CD1	6.34	124.80	121.00
2	B	29	G	O4'-C1'-N9	6.30	113.24	108.20
3	C	13	DT	C1'-O4'-C4'	-6.28	103.82	110.10
1	A	221	ARG	NE-CZ-NH1	6.25	123.43	120.30
2	B	3	C	O4'-C1'-N1	6.24	113.19	108.20
3	C	27	DG	O4'-C1'-C2'	-6.23	100.92	105.90
3	C	29	DC	P-O3'-C3'	6.23	127.17	119.70
2	B	85	C	O4'-C1'-N1	6.12	113.09	108.20
3	C	27	DG	C1'-O4'-C4'	-6.09	104.01	110.10
4	D	44	DT	C1'-O4'-C4'	-6.07	104.03	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	C	O4'-C1'-N1	6.03	113.03	108.20
2	B	20	G	O4'-C1'-N9	5.98	112.98	108.20
2	B	59	U	O4'-C1'-N1	5.98	112.98	108.20
2	B	1	U	O4'-C1'-N1	5.85	112.88	108.20
2	B	95	G	O4'-C1'-N9	5.75	112.80	108.20
2	B	37	U	O4'-C1'-N1	5.71	112.77	108.20
2	B	12	U	O4'-C1'-N1	5.65	112.72	108.20
2	B	19	U	O4'-C1'-N1	5.61	112.68	108.20
2	B	11	G	O4'-C1'-N9	5.56	112.65	108.20
2	B	72	U	O4'-C1'-N1	5.54	112.63	108.20
1	A	425	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	B	31	U	O4'-C1'-N1	5.54	112.63	108.20
3	C	28	DA	C1'-O4'-C4'	-5.53	104.57	110.10
3	C	38	DT	C1'-O4'-C4'	-5.51	104.59	110.10
2	B	21	G	O4'-C1'-N9	5.47	112.58	108.20
2	B	23	U	O4'-C1'-N1	5.45	112.56	108.20
2	B	53	G	O4'-C1'-N9	5.44	112.55	108.20
2	B	7	U	O4'-C1'-N1	5.43	112.55	108.20
2	B	64	U	O4'-C1'-N1	5.43	112.55	108.20
2	B	22	U	O4'-C1'-N1	5.42	112.53	108.20
2	B	15	U	O4'-C1'-N1	5.41	112.53	108.20
2	B	24	U	O4'-C1'-N1	5.37	112.49	108.20
2	B	39	G	O4'-C1'-N9	5.36	112.49	108.20
3	C	26	DC	O4'-C1'-C2'	-5.35	101.62	105.90
2	B	54	G	O4'-C1'-N9	5.33	112.46	108.20
2	B	10	A	O4'-C1'-N9	5.29	112.43	108.20
2	B	71	U	O4'-C1'-N1	5.28	112.42	108.20
2	B	68	A	O4'-C1'-N9	5.27	112.41	108.20
2	B	73	G	O4'-C1'-N9	5.26	112.41	108.20
3	C	31	DG	C1'-O4'-C4'	-5.25	104.85	110.10
1	A	653	ARG	NE-CZ-NH1	5.23	122.92	120.30
3	C	20	DC	O4'-C1'-C2'	-5.21	101.74	105.90
2	B	97	U	O4'-C1'-N1	5.18	112.34	108.20
2	B	62	G	O4'-C1'-N9	5.17	112.33	108.20
1	A	671	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	B	35	A	O4'-C1'-N9	5.15	112.32	108.20
2	B	18	A	O4'-C1'-N9	5.12	112.30	108.20
2	B	87	G	O4'-C1'-N9	5.12	112.29	108.20
2	B	77	A	O4'-C1'-N9	5.10	112.28	108.20
1	A	976	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	B	79	G	O4'-C1'-N9	5.06	112.25	108.20
2	B	14	G	O4'-C1'-N9	5.01	112.21	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	ARG	Sidechain
1	A	976	ARG	Sidechain

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	11172	0	11351	134	0
2	B	2110	0	1065	51	0
3	C	843	0	464	10	0
4	D	832	0	463	49	0
5	A	2	0	0	0	0
5	D	1	0	0	0	0
All	All	14960	0	13343	135	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 5.

All (135) 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:1021:MET:CB	4:D:23:DT:O4	1.77	1.31
1:A:1021:MET:HB2	4:D:23:DT:O4	1.11	1.25
1:A:164:PHE:CA	2:B:19:U:OP1	1.85	1.24
1:A:164:PHE:HA	2:B:19:U:OP1	1.19	1.23
1:A:1021:MET:HB3	4:D:23:DT:C4	1.76	1.18
1:A:1021:MET:CB	4:D:23:DT:C4	2.27	1.18
1:A:1311:HIS:ND1	4:D:36:DG:N2	1.97	1.12
1:A:156:LEU:HG	2:B:47:A:OP1	1.54	1.06
1:A:45:LYS:CA	2:B:91:C:H41	1.68	1.05
1:A:474:THR:HB	2:B:59:U:O4	1.57	1.03
1:A:919:ARG:O	4:D:32:DT:H71	1.57	1.03
1:A:72:TYR:CE1	2:B:50:U:H5	1.76	1.02
1:A:1169:MET:SD	2:B:52:A:O2'	2.22	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:ARG:O	4:D:32:DT:C7	2.12	0.97
1:A:911:LEU:HB2	4:D:35:DT:O2	1.63	0.97
1:A:72:TYR:CE1	2:B:50:U:C5	2.54	0.95
1:A:44:LYS:O	2:B:91:C:C5	2.25	0.90
1:A:45:LYS:C	2:B:91:C:H41	1.77	0.88
1:A:1037:PHE:CB	4:D:21:DG:H1	1.89	0.85
1:A:163:LYS:O	2:B:19:U:OP1	1.95	0.85
1:A:1004:LEU:HD21	4:D:18:DA:C2	2.12	0.84
1:A:163:LYS:O	2:B:19:U:P	2.36	0.84
1:A:1037:PHE:HB2	4:D:21:DG:H1	1.45	0.80
1:A:44:LYS:HE2	2:B:92:G:O6	1.83	0.78
1:A:164:PHE:CD1	2:B:19:U:H5''	2.19	0.77
1:A:1021:MET:HG3	4:D:23:DT:C7	2.14	0.76
1:A:1037:PHE:CG	4:D:21:DG:N2	2.49	0.76
1:A:917:ILE:O	1:A:918:LYS:CB	2.33	0.76
1:A:72:TYR:CZ	2:B:50:U:H5	2.03	0.76
1:A:1021:MET:HG3	4:D:23:DT:H71	1.67	0.75
1:A:1169:MET:HA	2:B:52:A:C2	2.22	0.75
1:A:156:LEU:CG	2:B:47:A:OP1	2.33	0.75
1:A:1169:MET:HA	2:B:52:A:N3	2.01	0.74
1:A:908:LEU:HD22	4:D:36:DG:N3	2.01	0.74
1:A:911:LEU:HB2	4:D:35:DT:C2	2.24	0.73
1:A:72:TYR:CZ	2:B:50:U:C5	2.76	0.72
1:A:909:SER:HB2	4:D:36:DG:H5'	1.70	0.72
1:A:1004:LEU:CD2	4:D:18:DA:C2	2.73	0.71
1:A:163:LYS:O	2:B:19:U:OP2	2.10	0.70
1:A:45:LYS:CA	2:B:91:C:N4	2.51	0.70
1:A:1021:MET:HB2	4:D:23:DT:C4	2.04	0.70
1:A:75:ARG:NH1	2:B:19:U:C5	2.60	0.69
1:A:844:GLN:HB2	3:C:22:DT:OP2	1.93	0.69
1:A:908:LEU:HD23	4:D:36:DG:H1'	1.75	0.68
1:A:1004:LEU:HD21	4:D:18:DA:N3	2.09	0.68
1:A:45:LYS:C	2:B:91:C:N4	2.47	0.68
1:A:45:LYS:N	2:B:91:C:N4	2.42	0.68
1:A:164:PHE:C	2:B:19:U:OP1	2.33	0.65
1:A:44:LYS:HD2	2:B:92:G:N7	2.12	0.65
1:A:774:GLN:HB2	3:C:34:DG:H5''	1.79	0.64
1:A:1311:HIS:CB	4:D:36:DG:H22	2.11	0.63
1:A:908:LEU:HD13	4:D:36:DG:H21	1.62	0.63
1:A:45:LYS:N	2:B:91:C:H41	1.93	0.63
1:A:45:LYS:HA	2:B:91:C:H41	1.59	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:PHE:HB3	4:D:21:DG:N1	2.14	0.63
1:A:37:ASN:O	1:A:38:THR:OG1	2.15	0.62
1:A:1037:PHE:CD2	4:D:21:DG:N2	2.66	0.62
1:A:325:TYR:OH	2:B:45:U:OP1	2.10	0.62
1:A:1037:PHE:HB3	4:D:21:DG:H1	1.62	0.61
1:A:1311:HIS:HB3	4:D:36:DG:H22	1.64	0.61
1:A:31:LYS:HD3	2:B:83:C:H41	1.65	0.61
1:A:1037:PHE:CB	4:D:21:DG:N1	2.63	0.61
1:A:917:ILE:O	1:A:918:LYS:HB2	2.01	0.60
1:A:165:ARG:N	2:B:19:U:OP1	2.35	0.60
1:A:1021:MET:HG3	4:D:23:DT:C5	2.37	0.59
1:A:133:PRO:O	2:B:45:U:H5''	2.03	0.58
1:A:168:PHE:HD2	1:A:168:PHE:O	1.86	0.58
1:A:1037:PHE:CB	4:D:21:DG:H22	2.15	0.57
1:A:1040:SER:OG	4:D:21:DG:C6	2.58	0.56
1:A:908:LEU:CD2	4:D:36:DG:H1'	2.35	0.56
1:A:917:ILE:O	1:A:918:LYS:HB3	2.07	0.55
1:A:105:PHE:HE1	2:B:48:A:HO2'	1.54	0.54
1:A:163:LYS:C	2:B:19:U:OP1	2.46	0.54
1:A:168:PHE:CD2	1:A:168:PHE:O	2.61	0.54
1:A:156:LEU:CD2	2:B:47:A:OP1	2.55	0.54
1:A:1311:HIS:HA	4:D:36:DG:H1	1.73	0.53
1:A:1311:HIS:CG	4:D:36:DG:N2	2.75	0.53
1:A:31:LYS:HE3	1:A:42:SER:OG	2.10	0.52
1:A:44:LYS:NZ	2:B:92:G:N7	2.51	0.52
1:A:164:PHE:N	2:B:19:U:OP1	2.40	0.51
1:A:1311:HIS:ND1	4:D:36:DG:C2	2.76	0.51
1:A:474:THR:CB	2:B:59:U:O4	2.44	0.50
1:A:775:LYS:HG3	1:A:775:LYS:O	2.11	0.50
1:A:773:GLY:O	1:A:777:SER:N	2.44	0.50
1:A:775:LYS:HB3	3:C:33:DA:H5''	1.94	0.50
1:A:1021:MET:HB3	4:D:23:DT:N3	2.22	0.50
1:A:1003:LYS:HD3	4:D:20:DC:O2	2.12	0.49
1:A:81:TYR:HE1	2:B:59:U:O2	1.96	0.49
1:A:919:ARG:HD2	4:D:33:DC:N4	2.27	0.49
1:A:135:ILE:N	2:B:46:A:OP1	2.45	0.49
1:A:774:GLN:HB2	3:C:34:DG:OP1	2.13	0.49
1:A:473:ILE:HD12	1:A:473:ILE:C	2.33	0.48
1:A:844:GLN:CB	3:C:22:DT:OP2	2.61	0.48
2:B:12:U:H3'	2:B:13:C:H5''	1.94	0.48
1:A:310:THR:O	1:A:311:GLU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:GLU:OE1	1:A:766:GLU:N	2.47	0.47
1:A:44:LYS:C	2:B:91:C:C5	2.88	0.47
1:A:1100:VAL:HG22	2:B:67:C:N3	2.30	0.47
1:A:866:LYS:HE2	3:C:21:DA:C2	2.50	0.47
1:A:1004:LEU:CD2	4:D:18:DA:N3	2.77	0.46
1:A:156:LEU:HG	2:B:47:A:P	2.51	0.46
1:A:1004:LEU:HD21	4:D:18:DA:H2	1.74	0.46
1:A:474:THR:OG1	1:A:475:PRO:HD2	2.16	0.45
1:A:1021:MET:CG	4:D:23:DT:H71	2.41	0.45
1:A:1003:LYS:HB3	4:D:20:DC:O2	2.17	0.45
1:A:115:ARG:NH1	2:B:25:U:O2	2.49	0.45
1:A:1281:ILE:O	1:A:1281:ILE:HG22	2.16	0.45
1:A:465:MET:SD	1:A:482:VAL:HB	2.57	0.44
1:A:1311:HIS:CG	4:D:36:DG:H22	2.35	0.44
1:A:352:PHE:O	1:A:353:ASP:HB2	2.17	0.44
1:A:1356:TYR:HB2	2:B:81:G:N2	2.31	0.44
1:A:31:LYS:CE	1:A:42:SER:OG	2.65	0.44
1:A:472:THR:O	1:A:481:VAL:HG21	2.17	0.44
1:A:60:GLU:HB3	1:A:844:GLN:HA	2.00	0.43
1:A:1169:MET:CG	2:B:52:A:O2'	2.66	0.43
1:A:851:SER:OG	1:A:852:ILE:N	2.52	0.43
1:A:774:GLN:HB2	3:C:34:DG:C5'	2.48	0.43
1:A:71:ARG:HH12	3:C:20:DC:N4	2.16	0.43
1:A:911:LEU:CB	4:D:35:DT:O2	2.52	0.43
1:A:156:LEU:C	1:A:156:LEU:HD23	2.39	0.43
1:A:71:ARG:HD2	1:A:72:TYR:N	2.33	0.43
1:A:44:LYS:C	2:B:91:C:C4	2.93	0.42
1:A:919:ARG:O	4:D:32:DT:H73	2.11	0.42
1:A:844:GLN:HG3	3:C:22:DT:OP2	2.18	0.42
1:A:72:TYR:CZ	2:B:50:U:C6	3.07	0.42
1:A:919:ARG:CB	4:D:32:DT:H73	2.51	0.41
1:A:775:LYS:HB3	3:C:33:DA:C4'	2.50	0.41
1:A:982:HIS:NE2	4:D:34:DA:OP2	2.50	0.41
1:A:727:LEU:O	1:A:728:ALA:HB3	2.21	0.41
1:A:1311:HIS:HA	4:D:36:DG:N1	2.36	0.41
1:A:161:MET:HB2	1:A:419:LEU:HD21	2.03	0.41
1:A:75:ARG:NH1	2:B:19:U:H5	2.15	0.41
1:A:72:TYR:CE2	2:B:50:U:OP2	2.74	0.40
1:A:1361:ASP:OD1	1:A:1362:LEU:N	2.54	0.40
1:A:1004:LEU:HD22	4:D:18:DA:C2	2.53	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	1366/1368 (100%)	1301 (95%)	61 (4%)	4 (0%)	43 81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	353	ASP
1	A	918	LYS
1	A	1248	SER

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	1225/1225 (100%)	1224 (100%)	1 (0%)	94 96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1335	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	98/99 (98%)	20 (20%)	0

All (20) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	4	C
2	B	13	C
2	B	34	A
2	B	35	A
2	B	37	U
2	B	42	A
2	B	51	A
2	B	53	G
2	B	56	U
2	B	58	G
2	B	59	U
2	B	63	U
2	B	67	C
2	B	74	A
2	B	75	A
2	B	77	A
2	B	82	G
2	B	85	C
2	B	89	G
2	B	91	C

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 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.