Full wwPDB EM Validation Report ⓘ

Jun 3, 2024 – 11:19 PM JST

PDB ID	:	8WMM
EMDB ID	:	EMD-37656
Title	:	Structure of CbCas9-PcrIIC1 complex bound to 28-bp DNA substrate (20-nt complementary)
Authors	:	Zhang, S.; Lin, S.; Liu, J.J.G.
Deposited on	:	2023-10-04
Resolution	:	2.98 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*
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.

The following versions of software and data (see references ⓘ) were used in the production of this report:

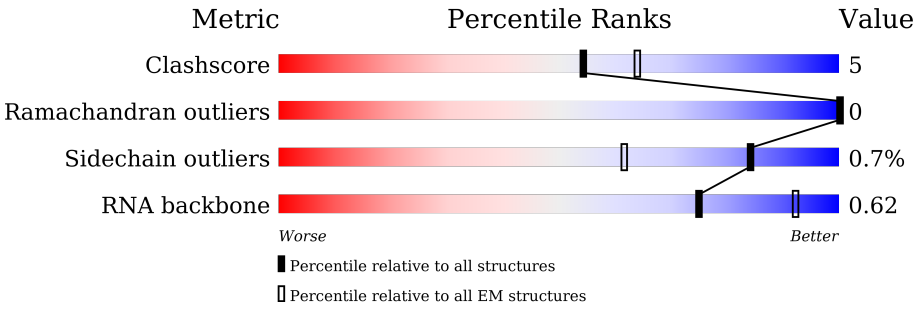
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.98 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	1442	73% 11% 16%
1	B	1442	73% 11% 16%
2	C	28	71% 29%
2	F	28	64% 36%
3	D	127	64% 19% . 14%
3	O	127	61% 20% 5% 14%
4	G	136	79% 19% .
4	H	136	78% 21% .

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Mol	Chain	Length	Quality of chain
5	S	28	36% 64%
5	Y	28	29% 7% 64%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28632 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 deadCbCas9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1212	Total	C	N	O	S	1	0
			10106	6459	1750	1878	19		
1	B	1212	Total	C	N	O	S	1	0
			10106	6459	1750	1878	19		

- Molecule 2 is a DNA chain called TS.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	28	Total	C	N	O	P	0	0
			561	269	88	176	28		
2	F	28	Total	C	N	O	P	0	0
			561	269	88	176	28		

- Molecule 3 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	109	Total	C	N	O	P	0	0
			2332	1043	422	758	109		
3	O	109	Total	C	N	O	P	0	0
			2332	1043	422	758	109		

- Molecule 4 is a protein called PcrIIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	134	Total	C	N	O	S	0	0
			1108	724	180	199	5		
4	H	134	Total	C	N	O	S	0	0
			1108	724	180	199	5		

- Molecule 5 is a DNA chain called NTS.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	10	Total	C	N	O	P	0	0
			208	98	46	54	10		
5	Y	10	Total	C	N	O	P	0	0
			208	98	46	54	10		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

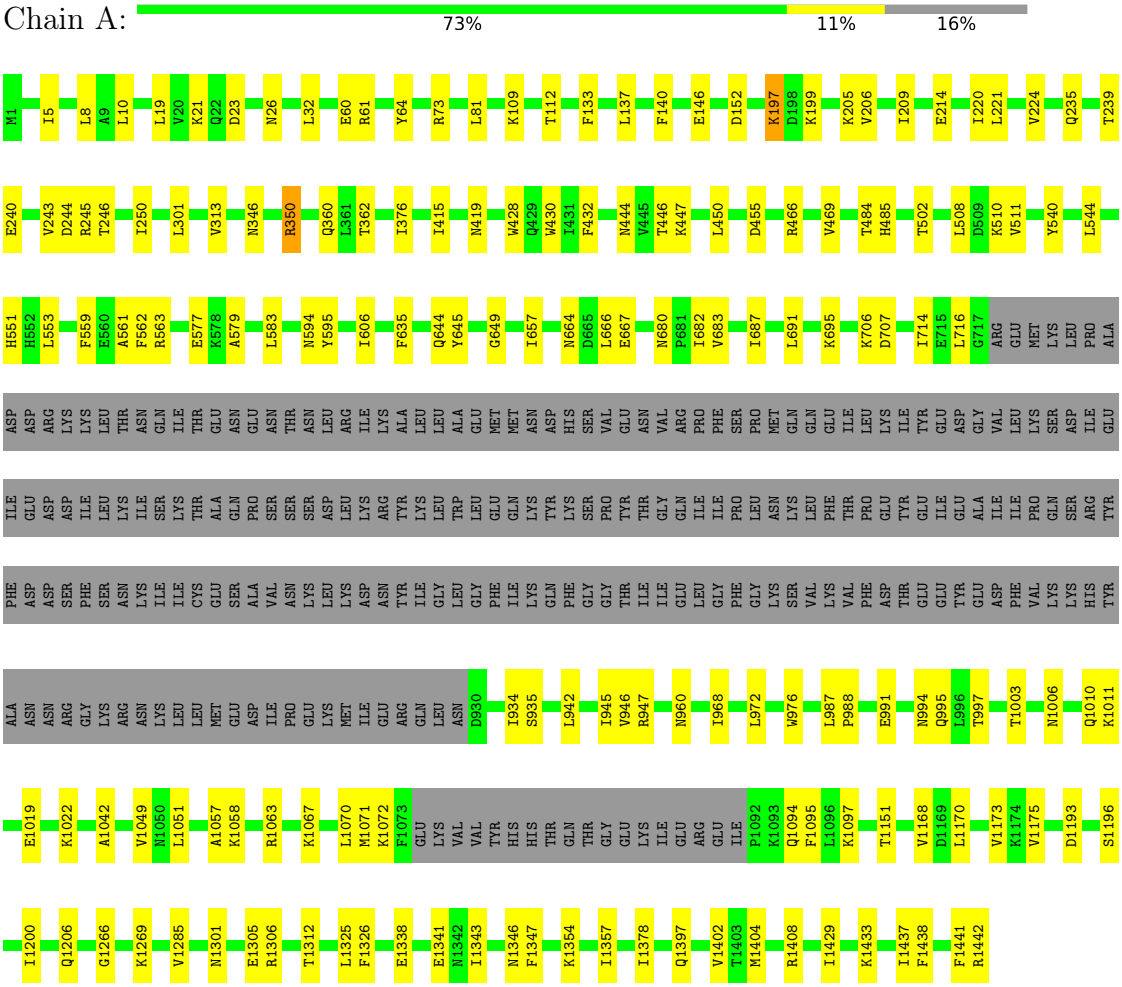
Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Mg	0
			1	1	
6	H	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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.

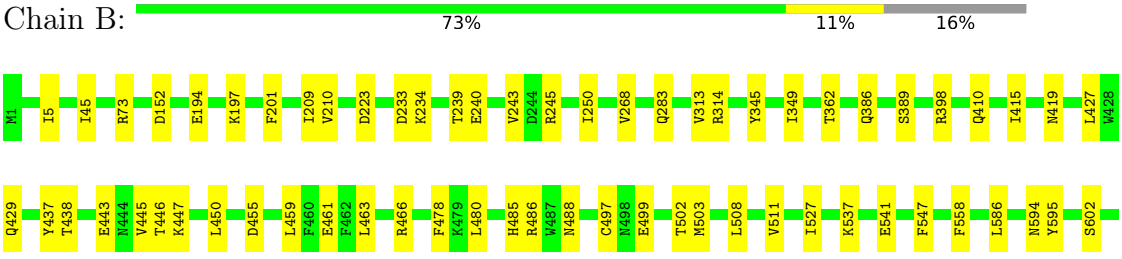
- Molecule 1: deadCbCas9

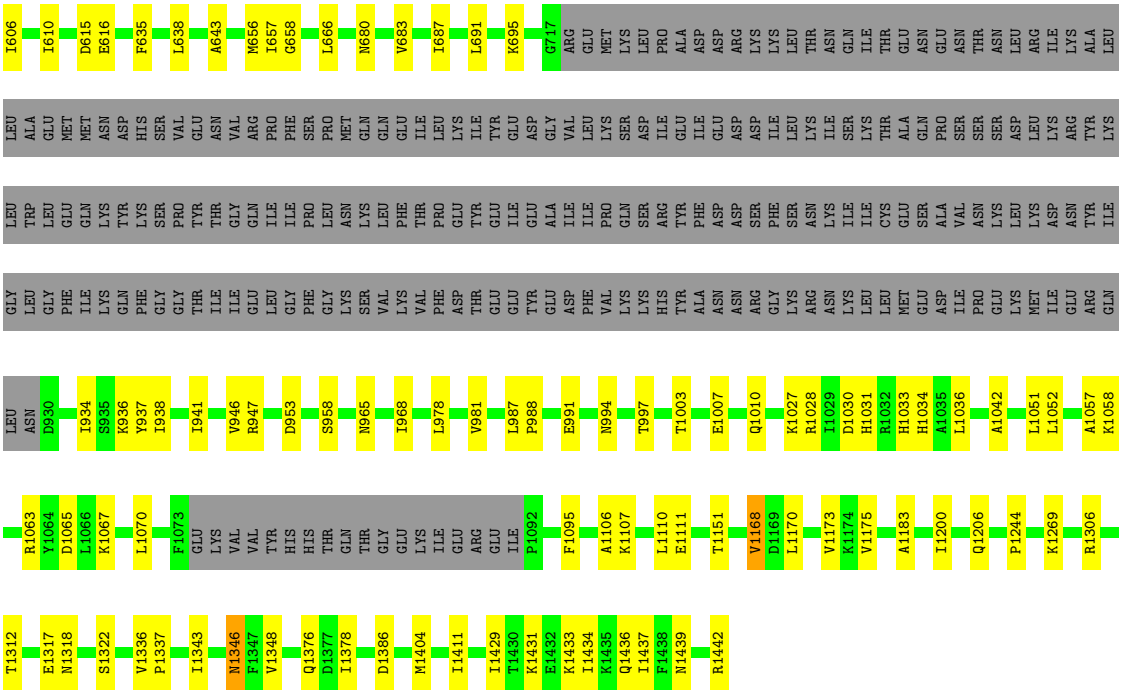
Chain A:



- Molecule 1: deadCbCas9

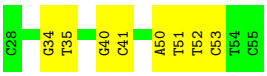
Chain B:





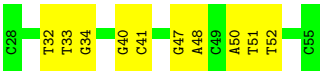
• Molecule 2: TS

Chain C:



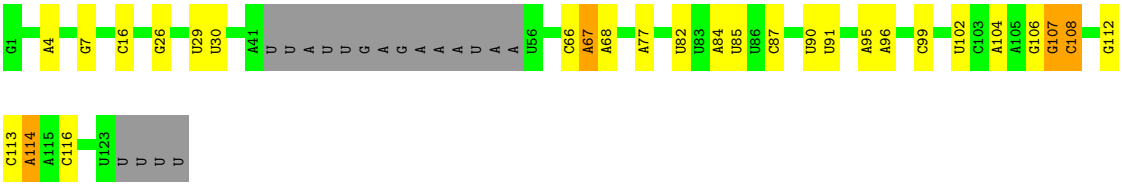
• Molecule 2: TS

Chain F:



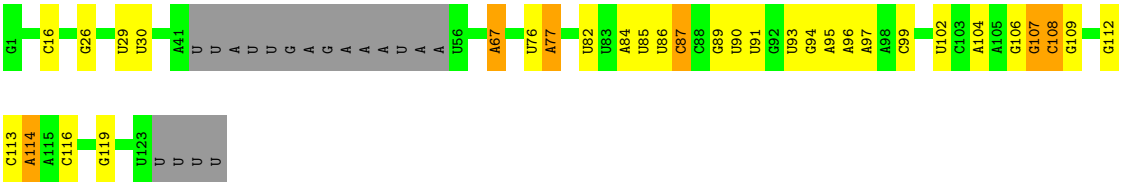
• Molecule 3: sgRNA

Chain D:



• Molecule 3: sgRNA

Chain O:



• Molecule 4: PcrIIC1

Chain G:

• Molecule 4: PcrIIC1

Chain H:

• Molecule 5: NTS

Chain S:

• Molecule 5: NTS

Chain Y:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	355919	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k 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: 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	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/10317	0.48	0/13871
1	B	0.27	0/10317	0.48	0/13871
2	C	0.43	0/623	0.76	0/957
2	F	0.42	0/623	0.75	0/957
3	D	0.28	0/2610	0.74	0/4064
3	O	0.27	0/2610	0.74	0/4064
4	G	0.31	0/1123	0.49	0/1511
4	H	0.30	0/1123	0.47	0/1511
5	S	0.49	0/235	0.72	0/360
5	Y	0.49	0/235	0.74	0/360
All	All	0.28	0/29816	0.56	0/41526

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

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	10106	0	10131	116	0
1	B	10106	0	10131	120	0
2	C	561	0	319	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	561	0	319	7	0
3	D	2332	0	1172	15	0
3	O	2332	0	1172	15	0
4	G	1108	0	1181	23	0
4	H	1108	0	1181	19	0
5	S	208	0	111	0	0
5	Y	208	0	111	1	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
All	All	28632	0	25828	293	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 (293) 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:B:1343:ILE:HG23	1:B:1346:ASN:HB3	1.68	0.76
1:B:1343:ILE:HG23	1:B:1346:ASN:CB	2.22	0.69
1:A:1051:LEU:HD21	1:A:1067:LYS:HE2	1.75	0.68
2:F:50:DA:H3'	2:F:51:DT:H71	1.76	0.67
1:A:1343:ILE:HG23	1:A:1346:ASN:CB	2.25	0.67
2:F:40:DG:H2"	2:F:41:DC:H5'	1.78	0.66
1:A:1343:ILE:HG23	1:A:1346:ASN:HB2	1.77	0.66
1:A:415:ILE:HD13	1:A:577:GLU:HB2	1.81	0.62
1:A:415:ILE:HD11	1:A:419:ASN:ND2	2.14	0.62
1:B:459:LEU:O	1:B:463:LEU:HD23	2.01	0.60
1:A:540:TYR:CE2	1:A:544:LEU:HD11	2.36	0.60
1:B:152:ASP:OD2	3:D:26:G:N2	2.35	0.59
1:B:1318:ASN:OD1	1:B:1322:SER:N	2.35	0.59
2:C:50:DA:H3'	2:C:51:DT:H71	1.84	0.59
1:B:981:VAL:HG13	1:B:1107:LYS:HD3	1.85	0.59
1:B:1051:LEU:HD22	1:B:1070:LEU:HD12	1.85	0.59
1:B:239:THR:O	1:B:243:VAL:HG13	2.02	0.59
4:H:9:ASP:OD1	4:H:10:THR:N	2.35	0.58
1:B:666:LEU:HD22	1:B:695:LYS:HB2	1.85	0.58
1:A:1051:LEU:HD22	1:A:1070:LEU:HD12	1.86	0.58
1:B:978:LEU:HD12	1:B:1036:LEU:HD11	1.84	0.58
1:B:73:ARG:NH2	3:D:16:C:OP1	2.32	0.58
1:A:666:LEU:HD22	1:A:695:LYS:HB2	1.84	0.58
1:A:250:ILE:O	1:A:250:ILE:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ASN:OD1	1:A:446:THR:HG22	2.03	0.58
2:F:51:DT:H2'	2:F:52:DT:C6	2.39	0.57
1:A:73:ARG:NH2	3:O:16:C:OP1	2.35	0.57
1:A:1301:ASN:O	1:A:1305:GLU:OE1	2.22	0.57
1:A:606:ILE:HG23	1:A:635:PHE:CE2	2.39	0.57
1:A:1402:VAL:HG21	1:A:1408:ARG:HG3	1.86	0.57
1:B:478:PHE:CB	1:B:480:LEU:HD13	2.34	0.56
1:B:586:LEU:HG	1:B:638:LEU:HD23	1.87	0.56
1:A:1306:ARG:NE	1:A:1312:THR:O	2.37	0.56
1:B:1429:ILE:O	1:B:1429:ILE:HG23	2.06	0.56
1:A:1266:GLY:O	1:A:1269:LYS:NZ	2.38	0.56
1:A:152:ASP:OD2	3:O:26:G:N2	2.39	0.55
1:A:994:ASN:ND2	1:A:1003:THR:OG1	2.39	0.55
1:B:965:ASN:OD1	1:B:968:ILE:HD12	2.07	0.55
1:A:1175:VAL:HG13	1:A:1175:VAL:O	2.07	0.55
1:A:484:THR:HG23	1:A:485:HIS:ND1	2.22	0.55
4:G:9:ASP:OD1	4:G:10:THR:N	2.35	0.55
1:B:1376:GLN:N	1:B:1376:GLN:OE1	2.38	0.55
1:A:645:TYR:O	1:A:649:GLY:N	2.35	0.54
1:A:687:ILE:HD11	1:A:934:ILE:HG22	1.89	0.54
1:A:243:VAL:O	1:A:245:ARG:NH1	2.41	0.54
1:B:937:TYR:CE2	1:B:941:ILE:HD11	2.42	0.54
1:B:1051:LEU:HD21	1:B:1067:LYS:HE2	1.89	0.54
1:A:1442:ARG:HD3	4:G:19:ASN:ND2	2.22	0.54
1:B:508:LEU:O	1:B:511:VAL:HG12	2.07	0.54
1:B:1030:ASP:OD1	1:B:1031:HIS:N	2.41	0.54
1:B:1168:VAL:HG23	3:D:66:C:H5"	1.90	0.54
1:A:579:ALA:O	1:A:583:LEU:HD23	2.08	0.53
1:B:313:VAL:HG23	1:B:313:VAL:O	2.08	0.53
1:B:586:LEU:HD23	1:B:643:ALA:HA	1.89	0.53
1:B:466:ARG:O	1:B:502:THR:OG1	2.25	0.53
1:B:478:PHE:HB2	1:B:480:LEU:HD13	1.90	0.53
1:B:656:MET:O	1:B:658:GLY:N	2.41	0.53
1:A:346:ASN:O	1:A:350:ARG:NE	2.41	0.52
1:B:606:ILE:O	1:B:610:ILE:HG12	2.10	0.52
1:A:313:VAL:HG23	1:A:313:VAL:O	2.10	0.52
1:B:1306:ARG:NE	1:B:1312:THR:O	2.41	0.52
1:A:559:PHE:O	1:A:563:ARG:N	2.40	0.52
3:D:107:G:O2'	3:D:108:C:OP1	2.28	0.52
3:O:107:G:HO2'	3:O:108:C:P	2.32	0.52
1:A:430:TRP:CH2	1:A:469:VAL:HG11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:107:G:O2'	3:D:108:C:P	2.68	0.51
3:O:107:G:O2'	3:O:108:C:P	2.67	0.51
1:A:199:LYS:O	1:A:250:ILE:HD11	2.11	0.51
1:B:981:VAL:HG13	1:B:1107:LYS:CD	2.41	0.50
1:B:1175:VAL:HG23	1:B:1175:VAL:O	2.12	0.50
1:A:10:LEU:HD23	1:A:714:ILE:HD11	1.93	0.50
1:A:209:ILE:O	1:A:209:ILE:HG13	2.10	0.50
1:A:133:PHE:CZ	1:A:137:LEU:HD21	2.46	0.50
1:B:437:TYR:O	1:B:486:ARG:N	2.39	0.50
1:B:362:THR:HG23	3:D:113:C:O2	2.11	0.50
1:A:214:GLU:N	1:A:220:ILE:HG23	2.27	0.50
1:A:1193:ASP:N	1:A:1196:SER:OG	2.44	0.49
4:H:18:ASP:OD1	4:H:19:ASN:N	2.45	0.49
1:B:594:ASN:OD1	1:B:595:TYR:N	2.44	0.49
1:A:972:LEU:HD23	1:A:1095:PHE:CD2	2.48	0.49
1:A:362:THR:HG23	3:O:113:C:O2	2.11	0.49
1:A:1433:LYS:O	1:A:1437:ILE:HG12	2.13	0.49
1:B:994:ASN:ND2	1:B:1003:THR:OG1	2.44	0.49
4:G:18:ASP:OD1	4:G:19:ASN:N	2.45	0.49
1:A:450:LEU:HD23	1:A:455:ASP:HB3	1.95	0.49
1:A:5:ILE:HG21	1:A:1042:ALA:O	2.12	0.49
1:A:209:ILE:HD11	1:A:239:THR:HG23	1.95	0.48
1:A:680:ASN:OD1	1:A:683:VAL:HG22	2.12	0.48
1:A:1343:ILE:HG23	1:A:1346:ASN:HB3	1.95	0.48
1:B:250:ILE:HD12	1:B:268:VAL:HG11	1.95	0.48
1:B:438:THR:HA	1:B:485:HIS:CD2	2.49	0.48
1:A:350:ARG:HG3	1:A:360:GLN:HE22	1.78	0.48
1:B:987:LEU:O	1:B:991:GLU:OE1	2.31	0.48
1:B:1336:VAL:HG21	1:B:1411:ILE:HD12	1.94	0.48
1:A:594:ASN:OD1	1:A:595:TYR:N	2.47	0.48
1:B:987:LEU:HG	1:B:991:GLU:OE2	2.14	0.48
1:A:1072:LYS:N	1:A:1094:GLN:O	2.43	0.48
3:O:107:G:O2'	3:O:108:C:OP1	2.30	0.48
1:A:205:LYS:HD2	1:A:246:THR:HG23	1.95	0.48
1:A:508:LEU:O	1:A:511:VAL:HG12	2.12	0.48
1:A:987:LEU:HG	1:A:991:GLU:OE2	2.13	0.48
1:B:1065:ASP:N	1:B:1065:ASP:OD1	2.47	0.48
1:B:1317:GLU:OE1	4:G:80:ARG:CB	2.63	0.47
1:A:1397:GLN:HE22	2:F:32:DT:H71	1.79	0.47
1:B:478:PHE:HB3	1:B:480:LEU:HD13	1.96	0.47
4:G:57:ASP:OD1	4:G:58:LYS:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:HIS:O	1:A:553:LEU:N	2.44	0.47
2:F:33:DT:H2"	2:F:34:DG:C8	2.50	0.47
1:A:976:TRP:HE1	1:A:1095:PHE:HB2	1.78	0.47
1:A:968:ILE:HD13	1:A:1049:VAL:HG12	1.96	0.47
1:B:429:GLN:NE2	3:D:4:A:O2'	2.45	0.47
1:B:438:THR:HG22	1:B:443:GLU:H	1.79	0.47
1:B:1007:GLU:O	1:B:1010:GLN:OE1	2.32	0.47
1:B:1336:VAL:HG21	1:B:1411:ILE:CD1	2.44	0.47
1:B:1433:LYS:O	1:B:1437:ILE:HG12	2.15	0.47
4:G:119:MET:O	4:G:119:MET:HG2	2.15	0.47
4:H:57:ASP:OD1	4:H:58:LYS:N	2.47	0.47
1:A:1071:MET:HG2	1:A:1095:PHE:CD1	2.50	0.47
4:G:11:ASN:ND2	4:G:116:SER:OG	2.47	0.47
4:H:11:ASN:ND2	4:H:116:SER:OG	2.47	0.47
1:A:544:LEU:HD21	1:A:562:PHE:HB3	1.97	0.46
1:B:233:ASP:OD1	1:B:234:LYS:N	2.49	0.46
1:A:706:LYS:O	1:A:707:ASP:OD1	2.34	0.46
1:B:1317:GLU:OE2	4:G:80:ARG:CB	2.64	0.46
1:B:209:ILE:HG13	1:B:209:ILE:O	2.14	0.46
4:G:97:LEU:CD1	4:H:51:GLU:OE2	2.64	0.46
1:A:997:THR:HG22	1:A:997:THR:O	2.16	0.46
1:B:463:LEU:HD13	1:B:497:CYS:SG	2.56	0.46
3:D:107:G:HO2'	3:D:108:C:P	2.38	0.46
4:H:119:MET:O	4:H:119:MET:HG2	2.15	0.46
1:A:133:PHE:O	1:A:137:LEU:HD23	2.16	0.46
1:A:1019:GLU:O	1:A:1022:LYS:NZ	2.31	0.46
1:A:21:LYS:HB2	1:A:32:LEU:HD11	1.97	0.45
1:A:19:LEU:CD2	1:A:32:LEU:HD12	2.46	0.45
1:A:61:ARG:NH2	3:O:89:G:OP1	2.49	0.45
1:A:1057:ALA:O	1:A:1058:LYS:HB2	2.15	0.45
1:B:463:LEU:O	1:B:497:CYS:SG	2.74	0.45
1:B:968:ILE:HG13	1:B:1052:LEU:HD12	1.97	0.45
1:B:1036:LEU:HD13	1:B:1110:LEU:HD11	1.98	0.45
1:B:1168:VAL:HG11	1:B:1183:ALA:HB2	1.97	0.45
4:H:14:LEU:HD21	4:H:49:VAL:HG11	1.99	0.45
5:Y:15:DC:H2"	5:Y:16:DA:C8	2.51	0.45
1:A:221:LEU:O	1:A:235:GLN:NE2	2.49	0.45
1:A:362:THR:HG21	3:O:114:A:C2	2.52	0.45
1:B:978:LEU:HD12	1:B:1036:LEU:CD1	2.46	0.45
1:A:243:VAL:O	1:A:244:ASP:OD1	2.34	0.45
1:B:201:PHE:N	1:B:283:GLN:OE1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1151:THR:O	1:A:1151:THR:HG23	2.16	0.45
4:H:103:LEU:HD11	4:H:119:MET:SD	2.57	0.45
1:A:583:LEU:HD11	1:A:644:GLN:HA	1.99	0.45
1:A:1071:MET:HG2	1:A:1095:PHE:HD1	1.81	0.45
1:A:1338:GLU:N	1:A:1341:GLU:OE1	2.40	0.45
1:B:1170:LEU:HB2	1:B:1173:VAL:HG22	1.99	0.45
1:B:511:VAL:HG23	1:B:558:PHE:N	2.32	0.45
1:B:934:ILE:O	1:B:938:ILE:HG22	2.16	0.45
1:B:1151:THR:HG23	1:B:1151:THR:O	2.17	0.45
1:B:946:VAL:HG22	1:B:946:VAL:O	2.17	0.44
1:B:1378:ILE:HD11	1:B:1404:MET:HE1	1.99	0.44
2:C:50:DA:C6	3:D:7:G:C6	3.05	0.44
1:A:987:LEU:O	1:A:991:GLU:OE1	2.35	0.44
1:B:537:LYS:O	1:B:541:GLU:OE1	2.35	0.44
1:B:1317:GLU:OE2	4:G:80:ARG:HB2	2.17	0.44
2:F:47:DG:H2'	2:F:48:DA:H8	1.83	0.44
1:B:586:LEU:HD23	1:B:643:ALA:CB	2.47	0.44
2:C:52:DT:H2'	2:C:53:DC:C6	2.53	0.44
1:A:109:LYS:O	1:A:112:THR:OG1	2.23	0.44
1:A:140:PHE:CD1	1:A:301:LEU:HD23	2.51	0.44
1:B:415:ILE:HD11	1:B:419:ASN:ND2	2.33	0.44
4:G:14:LEU:HD21	4:G:49:VAL:HG11	1.99	0.44
4:G:97:LEU:HD13	4:H:51:GLU:OE2	2.18	0.44
4:H:14:LEU:HD23	4:H:46:PHE:CE1	2.53	0.44
1:B:1107:LYS:O	1:B:1111:GLU:HG2	2.17	0.44
4:G:103:LEU:HD11	4:G:119:MET:SD	2.57	0.44
1:B:1057:ALA:O	1:B:1058:LYS:HB2	2.17	0.44
4:G:14:LEU:HD23	4:G:46:PHE:CE1	2.53	0.44
1:A:240:GLU:O	1:A:245:ARG:NH2	2.51	0.43
1:A:942:LEU:HD13	1:A:945:ILE:HD12	1.99	0.43
1:B:1244:PRO:O	3:D:30:U:O2'	2.36	0.43
1:B:1436:GLN:HA	1:B:1439:ASN:HB3	1.99	0.43
2:C:50:DA:N6	3:D:7:G:O6	2.50	0.43
1:A:81:LEU:CD2	1:A:376:ILE:HG21	2.48	0.43
1:A:209:ILE:CD1	1:A:239:THR:HG23	2.48	0.43
1:B:1033:HIS:CE1	1:B:1034:HIS:NE2	2.87	0.43
4:H:17:TYR:OH	4:H:56:MET:SD	2.66	0.43
1:A:197:LYS:HD2	1:A:197:LYS:O	2.17	0.43
1:A:1378:ILE:HD11	1:A:1404:MET:HE1	1.99	0.43
1:B:446:THR:O	1:B:447:LYS:HB3	2.19	0.43
1:A:510:LYS:HE3	1:A:561:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1051:LEU:HD12	1:B:1063:ARG:HH11	1.84	0.43
1:B:5:ILE:HG21	1:B:1042:ALA:O	2.18	0.43
1:B:635:PHE:HA	1:B:638:LEU:HD21	2.00	0.43
1:A:946:VAL:O	1:A:946:VAL:HG22	2.18	0.43
1:B:1343:ILE:HG23	1:B:1346:ASN:HB2	1.99	0.43
1:A:8:LEU:HB2	1:A:714:ILE:HD12	2.01	0.43
1:B:527:ILE:HD11	1:B:547:PHE:CZ	2.53	0.43
1:A:466:ARG:O	1:A:502:THR:OG1	2.36	0.43
1:A:657:ILE:CG2	1:A:947:ARG:HD3	2.48	0.43
1:A:987:LEU:N	1:A:988:PRO:HD2	2.34	0.43
1:A:1170:LEU:HB2	1:A:1173:VAL:HG22	2.01	0.43
1:B:194:GLU:HB3	1:B:197:LYS:HE3	2.00	0.43
1:B:1337:PRO:HB3	1:B:1343:ILE:CG1	2.48	0.43
1:A:446:THR:O	1:A:447:LYS:HB3	2.17	0.43
1:A:1347:PHE:CD1	1:A:1347:PHE:N	2.85	0.43
1:A:428:TRP:O	1:A:432:PHE:CD2	2.72	0.43
1:B:1348:VAL:O	1:B:1348:VAL:HG13	2.18	0.43
1:A:682:ILE:HD12	1:A:682:ILE:H	1.84	0.42
1:A:1051:LEU:HD12	1:A:1063:ARG:NH1	2.33	0.42
1:A:206:VAL:HG13	1:A:224:VAL:HG13	2.00	0.42
1:A:687:ILE:O	1:A:691:LEU:HD23	2.19	0.42
1:B:657:ILE:CG2	1:B:947:ARG:HD3	2.49	0.42
1:A:946:VAL:O	1:A:960:ASN:ND2	2.52	0.42
1:B:934:ILE:H	1:B:934:ILE:HD12	1.84	0.42
1:B:997:THR:HG22	1:B:997:THR:O	2.19	0.42
3:D:29:U:O2'	3:D:30:U:H5'	2.19	0.42
4:H:126:ASP:HB3	4:H:128:LYS:HD2	2.01	0.42
1:A:81:LEU:HD23	1:A:376:ILE:HG21	2.01	0.42
4:H:11:ASN:OD1	4:H:12:ILE:N	2.52	0.42
1:B:445:VAL:HG22	1:B:445:VAL:O	2.19	0.42
1:B:488:ASN:OD1	1:B:488:ASN:O	2.38	0.42
1:B:953:ASP:OD2	1:B:958:SER:OG	2.24	0.42
1:B:1106:ALA:O	1:B:1110:LEU:HG	2.19	0.42
1:A:1354:LYS:HA	1:A:1357:ILE:HG22	2.02	0.42
1:A:1168:VAL:HG11	3:O:67:A:OP1	2.20	0.42
1:A:1285:VAL:O	1:A:1325:LEU:N	2.52	0.42
1:A:1325:LEU:HG	1:A:1326:PHE:CD2	2.55	0.42
1:B:1200:ILE:O	1:B:1206:GLN:NE2	2.51	0.42
1:A:23:ASP:OD2	1:A:26:ASN:ND2	2.52	0.42
1:B:239:THR:O	1:B:243:VAL:HG22	2.20	0.42
1:B:450:LEU:HD23	1:B:455:ASP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1028:ARG:HD2	1:B:1028:ARG:O	2.20	0.42
1:B:1431:LYS:O	1:B:1434:ILE:HG22	2.20	0.42
2:F:40:DG:H2"	2:F:41:DC:C5'	2.49	0.42
1:A:60:GLU:HG2	1:A:64:TYR:CE2	2.54	0.42
1:B:1027:LYS:HE2	1:B:1033:HIS:HB2	2.02	0.42
1:B:240:GLU:O	1:B:245:ARG:NH1	2.52	0.41
4:G:126:ASP:HB3	4:G:128:LYS:HD2	2.01	0.41
3:O:29:U:O2'	3:O:30:U:H5'	2.20	0.41
1:A:1438:PHE:HE1	4:G:16:ALA:O	2.04	0.41
1:A:1441:PHE:CE2	4:G:64:LEU:HD13	2.54	0.41
1:B:1051:LEU:HD12	1:B:1063:ARG:NH1	2.35	0.41
2:C:34:DG:C5	2:C:35:DT:C4	3.09	0.41
4:G:11:ASN:OD1	4:G:12:ILE:N	2.52	0.41
4:G:119:MET:HG2	4:G:131:ILE:HD13	2.02	0.41
1:A:976:TRP:HA	1:A:1097:LYS:HE2	2.02	0.41
1:A:1438:PHE:HB3	4:G:64:LEU:HD21	2.03	0.41
1:B:197:LYS:HE2	1:B:197:LYS:HA	2.02	0.41
1:B:386:GLN:O	1:B:389:SER:OG	2.34	0.41
1:B:427:LEU:HD11	1:B:463:LEU:HD12	2.02	0.41
1:B:680:ASN:OD1	1:B:683:VAL:HG22	2.21	0.41
1:B:45:ILE:HD12	1:B:45:ILE:H	1.84	0.41
1:B:463:LEU:CD1	1:B:497:CYS:SG	3.08	0.41
1:B:602:SER:O	1:B:606:ILE:HG13	2.20	0.41
4:H:4:ASP:OD1	4:H:4:ASP:N	2.53	0.41
1:A:205:LYS:CD	1:A:246:THR:HG23	2.50	0.41
1:A:1200:ILE:O	1:A:1206:GLN:NE2	2.53	0.41
1:A:1429:ILE:HD12	1:A:1433:LYS:HG2	2.03	0.41
1:B:987:LEU:N	1:B:988:PRO:HD2	2.36	0.41
1:B:937:TYR:CZ	1:B:941:ILE:HD11	2.56	0.41
3:O:76:U:O3'	3:O:77:A:H4'	2.21	0.41
3:O:93:U:H2'	3:O:94:G:O4'	2.20	0.41
1:B:615:ASP:OD1	1:B:616:GLU:N	2.54	0.41
1:B:934:ILE:O	1:B:934:ILE:HG22	2.20	0.41
1:B:1429:ILE:HB	4:H:71:GLU:OE2	2.19	0.41
2:C:40:DG:H2"	2:C:41:DC:H5'	2.01	0.41
4:H:119:MET:HG2	4:H:131:ILE:HD13	2.02	0.41
1:A:968:ILE:O	1:A:972:LEU:HG	2.21	0.41
1:A:1010:GLN:HA	1:A:1010:GLN:OE1	2.20	0.41
1:B:497:CYS:SG	1:B:497:CYS:O	2.78	0.41
1:B:1052:LEU:HD11	1:B:1095:PHE:CZ	2.56	0.41
3:O:109:G:C6	3:O:119:G:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ILE:HD11	1:A:419:ASN:HD22	1.86	0.40
1:B:362:THR:HG21	3:D:114:A:C2	2.56	0.40
1:B:687:ILE:O	1:B:691:LEU:HD23	2.21	0.40
1:B:1051:LEU:HD11	1:B:1067:LYS:CE	2.52	0.40
1:B:1317:GLU:OE1	4:G:80:ARG:HG2	2.22	0.40
1:B:1386:ASP:OD1	1:B:1386:ASP:N	2.54	0.40
4:H:12:ILE:HD13	4:H:135:PHE:CE1	2.56	0.40
3:O:86:U:H2'	3:O:87:C:O4'	2.20	0.40
1:A:1429:ILE:HD12	1:A:1433:LYS:CG	2.51	0.40
1:B:345:TYR:CE2	1:B:349:ILE:HD11	2.57	0.40
1:A:664:ASN:O	1:A:667:GLU:HG2	2.21	0.40
1:A:716:LEU:HD22	1:A:935:SER:OG	2.22	0.40
1:A:1438:PHE:CZ	4:G:16:ALA:HB1	2.57	0.40
1:B:210:VAL:N	1:B:223:ASP:OD1	2.54	0.40
1:B:398:ARG:HB2	1:B:410:GLN:CG	2.52	0.40
1:B:499:GLU:O	1:B:503:MET:HG3	2.22	0.40
4:G:12:ILE:HD13	4:G:135:PHE:CE1	2.56	0.40
1:A:1006:ASN:OD1	1:A:1011:LYS:O	2.40	0.40
1:B:1442:ARG:HD3	4:H:17:TYR:O	2.21	0.40
3:D:67:A:H2'	3:D:68:A:C8	2.56	0.40
3:D:82:U:O2	3:D:84:A:N1	2.54	0.40
4:H:6:ILE:HD11	4:H:115:LEU:HD21	2.03	0.40
3:O:82:U:O2	3:O:84:A:N1	2.55	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	1207/1442 (84%)	1143 (95%)	64 (5%)	0	100	100
1	B	1207/1442 (84%)	1146 (95%)	61 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	G	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
4	H	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
All	All	2678/3156 (85%)	2543 (95%)	135 (5%)	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	1116/1328 (84%)	1112 (100%)	4 (0%)	91	97
1	B	1116/1328 (84%)	1110 (100%)	6 (0%)	88	95
4	G	129/131 (98%)	125 (97%)	4 (3%)	40	73
4	H	129/131 (98%)	126 (98%)	3 (2%)	50	79
All	All	2490/2918 (85%)	2473 (99%)	17 (1%)	84	93

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	197	LYS
1	A	350	ARG
1	A	995	GLN
1	B	314	ARG
1	B	461	GLU
1	B	936	LYS
1	B	1168	VAL
1	B	1269	LYS
1	B	1346	ASN
4	G	26	ASP
4	G	52	ARG
4	G	71	GLU
4	G	73	ILE

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Mol	Chain	Res	Type
4	H	26	ASP
4	H	52	ARG
4	H	73	ILE

Sometimes 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
3	D	107/127 (84%)	16 (14%)	1 (0%)
3	O	107/127 (84%)	17 (15%)	1 (0%)
All	All	214/254 (84%)	33 (15%)	2 (0%)

All (33) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	D	67	A
3	D	77	A
3	D	85	U
3	D	87	C
3	D	90	U
3	D	91	U
3	D	95	A
3	D	96	A
3	D	99	C
3	D	102	U
3	D	104	A
3	D	106	G
3	D	108	C
3	D	112	G
3	D	114	A
3	D	116	C
3	O	67	A
3	O	77	A
3	O	85	U
3	O	87	C
3	O	90	U
3	O	91	U
3	O	95	A
3	O	96	A

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Mol	Chain	Res	Type
3	O	97	A
3	O	99	C
3	O	102	U
3	O	104	A
3	O	106	G
3	O	108	C
3	O	112	G
3	O	114	A
3	O	116	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	107	G
3	O	107	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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.