



## Full wwPDB EM Validation Report ⓘ

Apr 27, 2025 – 03:53 AM JST

PDB ID : 8ZTY / pdb\_00008zty  
EMDB ID : EMD-60476  
Title : Cryo-EM structure of the Cas13a-rAcrVIA1 complex  
Authors : Zhang, J.T.; Li, Y.L.; Jia, N.  
Deposited on : 2024-06-07  
Resolution : 2.85 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

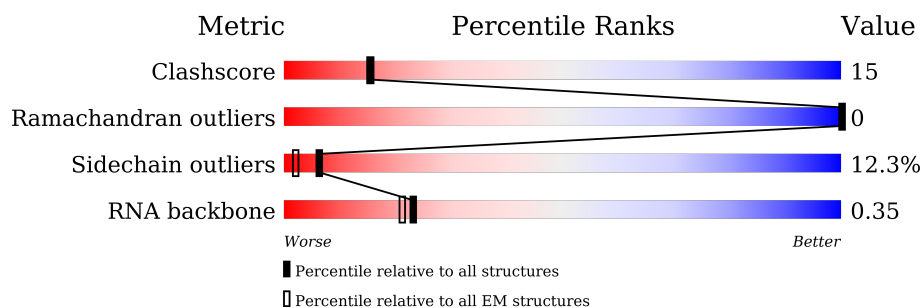
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*



The reported resolution of this entry is 2.85 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1120	
2	B	65	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8923 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 endoribonuclease Cas13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	928	Total	C	N	O	S	0	0
			7712	4927	1311	1447	27		

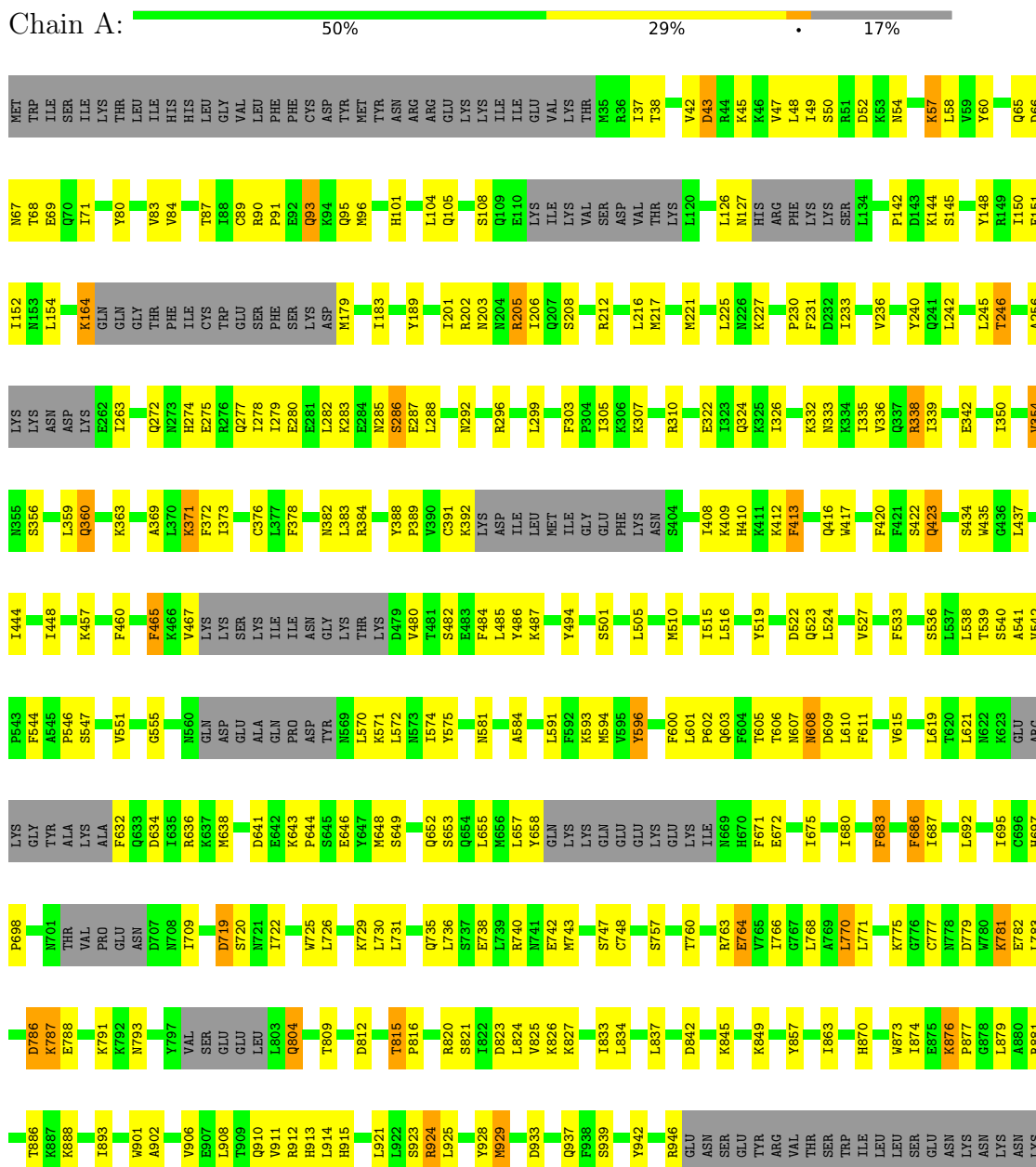
- Molecule 2 is a RNA chain called rAcrVIA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	57	Total	C	N	O	P	0	0
			1211	543	218	394	56		

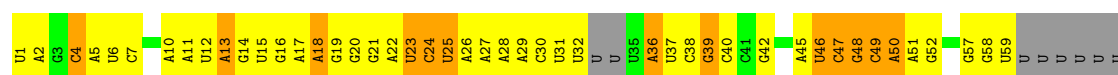
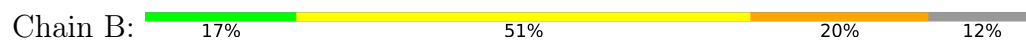
### 3 Residue-property plots

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: CRISPR-associated endoribonuclease Cas13a



- Molecule 2: rAcrVIA1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	451586	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0/7851	0.52	2/10538 (0.0%)
2	B	0.18	0/1353	0.76	0/2104
All	All	0.25	0/9204	0.57	2/12642 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	PRO	CA-N-CD	-7.76	100.64	111.50
1	A	43	ASP	CB-CG-OD2	6.93	124.54	118.30

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	A	7712	0	7750	232	0
2	B	1211	0	617	42	0
All	All	8923	0	8367	251	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 15.

All (251) 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:1060:GLU:HG2	2:B:28:A:H5''	1.66	0.78
1:A:1041:ARG:HE	1:A:1051:LYS:HZ3	1.31	0.76
1:A:505:LEU:HD21	1:A:775:LYS:HE3	1.68	0.75
1:A:740:ARG:HB2	1:A:766:ILE:HG21	1.67	0.75
1:A:603:GLN:O	1:A:607:ASN:HB3	1.87	0.74
1:A:150:ILE:HD12	1:A:151:GLU:H	1.51	0.74
1:A:914:LEU:HD11	1:A:1112:LEU:HD23	1.71	0.72
1:A:540:SER:H	1:A:763:ARG:HH12	1.38	0.71
1:A:600:PHE:HD1	1:A:601:LEU:HD23	1.56	0.69
1:A:740:ARG:HH12	1:A:770:LEU:HG	1.57	0.69
1:A:126:LEU:HD21	1:A:154:LEU:HD12	1.75	0.68
1:A:57:LYS:HG2	1:A:66:ASP:HB3	1.76	0.67
1:A:821:SER:HB3	1:A:911:VAL:HB	1.75	0.67
1:A:575:TYR:HE2	1:A:680:ILE:HG23	1.57	0.67
1:A:596:TYR:HE2	1:A:601:LEU:HD21	1.58	0.67
1:A:600:PHE:CD1	1:A:601:LEU:HD23	2.29	0.67
1:A:901:TRP:NE1	1:A:1108:GLU:OE1	2.26	0.66
2:B:6:U:H2'	2:B:7:C:C6	2.33	0.64
1:A:413:PHE:HE2	1:A:434:SER:HB3	1.63	0.63
1:A:672:GLU:OE2	2:B:29:A:O2'	2.16	0.63
1:A:275:GLU:OE2	1:A:292:ASN:ND2	2.33	0.62
1:A:541:ALA:H	1:A:605:THR:HG21	1.65	0.62
1:A:417:TRP:HE1	1:A:494:TYR:HE2	1.47	0.61
1:A:655:LEU:HD13	1:A:671:PHE:HB2	1.82	0.61
1:A:921:LEU:HD13	1:A:1033:ILE:HG21	1.82	0.61
1:A:1044:LEU:HD13	1:A:1050:LEU:HB3	1.81	0.61
1:A:924:ARG:HH12	2:B:27:A:H5'	1.65	0.61
1:A:501:SER:O	1:A:505:LEU:N	2.30	0.60
1:A:409:LYS:HG2	1:A:412:LYS:HE2	1.82	0.60
1:A:363:LYS:NZ	2:B:26:A:OP2	2.22	0.59
1:A:538:LEU:HD21	1:A:760:THR:HG23	1.82	0.59
1:A:547:SER:N	2:B:31:U:OP1	2.32	0.59
1:A:731:LEU:HB2	1:A:736:LEU:HG	1.85	0.59
1:A:823:ASP:OD2	1:A:824:LEU:N	2.35	0.59
1:A:519:TYR:HE2	1:A:695:ILE:HG23	1.68	0.59
1:A:1069:VAL:HB	1:A:1086:LEU:HD12	1.84	0.59
1:A:527:VAL:HB	1:A:692:LEU:HD21	1.85	0.58
1:A:874:ILE:HG13	2:B:39:G:C2	2.38	0.58
1:A:608:ASN:HB3	1:A:644:PRO:HD3	1.85	0.58
1:A:279:ILE:HA	1:A:282:LEU:HG	1.85	0.58
1:A:653:SER:O	1:A:657:LEU:HD13	2.03	0.58
1:A:225:LEU:HD12	1:A:946:ARG:HE	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:G:N1	2:B:58:G:O6	2.36	0.57
1:A:643:LYS:HB2	1:A:646:GLU:HG3	1.86	0.57
1:A:779:ASP:HB3	1:A:783:LEU:HB2	1.86	0.57
1:A:383:LEU:HD13	1:A:437:LEU:HB3	1.86	0.57
1:A:389:PRO:O	1:A:1026:ASN:ND2	2.38	0.57
1:A:824:LEU:HD21	1:A:915:HIS:CD2	2.40	0.57
2:B:25:U:H2'	2:B:26:A:C8	2.39	0.57
1:A:516:LEU:HD11	1:A:709:ILE:HD11	1.87	0.57
1:A:413:PHE:CE2	1:A:434:SER:HB3	2.40	0.56
1:A:837:LEU:HD22	1:A:1116:LEU:HB2	1.86	0.56
1:A:208:SER:O	1:A:338:ARG:NH2	2.38	0.56
1:A:279:ILE:HG13	1:A:283:LYS:HG3	1.88	0.56
1:A:510:MET:HG3	1:A:515:ILE:HD13	1.88	0.55
1:A:37:ILE:N	2:B:21:G:OP1	2.40	0.55
1:A:1038:ASP:OD2	1:A:1080:HIS:ND1	2.40	0.54
1:A:596:TYR:CE2	1:A:601:LEU:HD21	2.41	0.53
1:A:648:MET:CE	1:A:675:ILE:HG13	2.38	0.53
1:A:307:LYS:HA	2:B:48:G:C5	2.43	0.53
1:A:929:MET:HE1	1:A:1040:ALA:HA	1.90	0.53
1:A:1090:LYS:HB3	1:A:1101:SER:HB2	1.90	0.53
1:A:815:THR:O	1:A:815:THR:OG1	2.18	0.53
1:A:538:LEU:HD12	1:A:538:LEU:H	1.72	0.53
1:A:1039:ASP:O	1:A:1043:VAL:HG12	2.09	0.53
1:A:50:SER:HA	1:A:356:SER:HB3	1.91	0.53
1:A:804:GLN:O	1:A:809:THR:OG1	2.27	0.53
2:B:4:C:H42	2:B:50:A:H2	1.57	0.53
2:B:6:U:H2'	2:B:7:C:H6	1.73	0.53
1:A:1015:LYS:O	1:A:1019:ILE:HG22	2.09	0.52
1:A:278:ILE:HG23	1:A:282:LEU:HD23	1.90	0.52
1:A:65:GLN:O	1:A:67:ASN:ND2	2.43	0.52
1:A:360:GLN:HG3	2:B:23:U:C2	2.45	0.52
2:B:39:G:H2'	2:B:40:C:C6	2.45	0.52
1:A:467:VAL:HB	1:A:482:SER:HB2	1.92	0.52
1:A:902:ALA:O	1:A:906:VAL:HG22	2.09	0.52
1:A:570:LEU:HB3	1:A:572:LEU:HD13	1.92	0.51
1:A:1041:ARG:HH12	1:A:1055:SER:HB2	1.75	0.51
1:A:1052:ASN:ND2	2:B:5:A:O2'	2.43	0.51
1:A:58:LEU:HG	1:A:201:ILE:HG21	1.93	0.51
1:A:80:TYR:HE1	1:A:104:LEU:HB3	1.75	0.51
1:A:485:LEU:HB3	1:A:487:LYS:HZ3	1.75	0.51
1:A:873:TRP:CD1	1:A:877:PRO:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:TYR:HE2	1:A:1033:ILE:HG13	1.76	0.51
1:A:1041:ARG:HH22	1:A:1055:SER:HB2	1.75	0.51
1:A:47:VAL:HG21	1:A:71:ILE:HG21	1.91	0.51
1:A:203:ASN:ND2	2:B:10:A:OP1	2.43	0.51
1:A:575:TYR:CE2	1:A:680:ILE:HG23	2.44	0.51
1:A:510:MET:SD	1:A:524:LEU:HD21	2.52	0.50
1:A:541:ALA:N	1:A:605:THR:HG21	2.27	0.50
1:A:69:GLU:N	1:A:69:GLU:OE1	2.45	0.50
1:A:933:ASP:O	1:A:937:GLN:HG2	2.12	0.50
1:A:505:LEU:HD11	1:A:775:LYS:HG3	1.93	0.50
1:A:649:SER:O	1:A:652:GLN:HG3	2.11	0.50
2:B:46:U:O2'	2:B:47:C:O5'	2.24	0.50
1:A:179:MET:O	1:A:183:ILE:HG12	2.12	0.49
1:A:1033:ILE:HB	1:A:1117:LEU:HD13	1.94	0.49
1:A:230:PRO:HG2	1:A:231:PHE:CE1	2.47	0.49
2:B:28:A:H2'	2:B:29:A:C8	2.47	0.49
2:B:58:G:H2'	2:B:59:U:C6	2.47	0.49
1:A:1044:LEU:HD22	1:A:1050:LEU:HD13	1.94	0.49
1:A:1109:TYR:HD1	1:A:1109:TYR:O	1.95	0.49
1:A:93:GLN:NE2	1:A:96:MET:HB2	2.27	0.49
1:A:581:ASN:HD21	1:A:863:ILE:HB	1.77	0.49
1:A:608:ASN:OD1	1:A:608:ASN:N	2.45	0.49
1:A:657:LEU:HD12	2:B:23:U:H5'	1.94	0.49
1:A:540:SER:HB3	1:A:601:LEU:HB3	1.95	0.49
1:A:740:ARG:HH11	1:A:766:ILE:HG22	1.75	0.49
1:A:80:TYR:CE1	1:A:104:LEU:HB3	2.47	0.49
1:A:285:ASN:OD1	1:A:287:GLU:HG2	2.13	0.49
1:A:1072:LYS:HG3	1:A:1084:ASP:HB2	1.93	0.49
1:A:233:ILE:HA	1:A:236:VAL:HG12	1.93	0.49
1:A:465:PHE:HD2	1:A:484:PHE:HB2	1.77	0.49
1:A:279:ILE:HD11	2:B:13:A:C4	2.47	0.49
1:A:285:ASN:HD21	1:A:288:LEU:HD12	1.78	0.48
1:A:600:PHE:CE2	1:A:683:PHE:HA	2.48	0.48
1:A:256:ALA:HA	1:A:263:ILE:HD13	1.94	0.48
1:A:921:LEU:O	1:A:925:LEU:HD12	2.13	0.48
1:A:465:PHE:CD2	1:A:484:PHE:HB2	2.49	0.48
1:A:57:LYS:NZ	1:A:202:ARG:HG3	2.28	0.48
1:A:522:ASP:OD1	1:A:522:ASP:N	2.45	0.48
1:A:369:ALA:HA	1:A:448:ILE:HD11	1.95	0.48
1:A:417:TRP:HZ3	1:A:437:LEU:HD22	1.78	0.48
1:A:487:LYS:HG2	1:A:719:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:LEU:HD23	1:A:709:ILE:HD13	1.95	0.47
1:A:45:LYS:HG3	1:A:60:TYR:HD2	1.79	0.47
1:A:1049:LYS:HB3	2:B:6:U:O2'	2.15	0.47
1:A:1017:ASN:HA	1:A:1021:HIS:CE1	2.50	0.47
1:A:422:SER:O	1:A:422:SER:OG	2.26	0.47
1:A:1028:GLN:HG3	1:A:1029:LEU:HD12	1.97	0.47
1:A:384:ARG:NH1	1:A:389:PRO:O	2.48	0.47
1:A:54:ASN:HA	1:A:205:ARG:HH12	1.80	0.46
1:A:242:LEU:O	1:A:246:THR:OG1	2.30	0.46
1:A:908:LEU:HD13	1:A:911:VAL:HG21	1.96	0.46
1:A:216:LEU:HB2	1:A:286:SER:HB2	1.98	0.46
1:A:870:HIS:O	1:A:874:ILE:HD13	2.16	0.46
2:B:50:A:H2'	2:B:51:A:C8	2.50	0.46
1:A:245:LEU:HD12	1:A:274:HIS:HD1	1.80	0.46
1:A:782:GLU:H	1:A:782:GLU:HG2	1.60	0.46
1:A:1081:LEU:HD23	1:A:1081:LEU:H	1.81	0.46
1:A:725:TRP:CD1	1:A:768:LEU:HD23	2.51	0.46
1:A:371:LYS:HE3	1:A:371:LYS:HA	1.98	0.46
1:A:611:PHE:HZ	1:A:648:MET:SD	2.39	0.46
2:B:21:G:H2'	2:B:22:A:C8	2.51	0.46
1:A:296:ARG:NH1	2:B:17:A:O2'	2.48	0.46
1:A:437:LEU:HD12	1:A:437:LEU:HA	1.84	0.46
2:B:4:C:H5''	2:B:5:A:O4'	2.16	0.46
1:A:65:GLN:HG2	1:A:67:ASN:ND2	2.32	0.45
1:A:876:LYS:HG3	1:A:879:LEU:HG	1.99	0.45
2:B:46:U:H3	2:B:52:G:H1	1.64	0.45
2:B:48:G:N7	2:B:49:C:N4	2.65	0.45
1:A:89:CYS:SG	1:A:90:ARG:N	2.88	0.45
1:A:519:TYR:CE2	1:A:695:ILE:HG23	2.49	0.45
1:A:335:ILE:O	1:A:339:ILE:HG23	2.17	0.45
2:B:45:A:H2'	2:B:46:U:H5'	1.98	0.45
1:A:212:ARG:HG3	1:A:286:SER:HB3	1.98	0.45
1:A:544:PHE:O	1:A:546:PRO:HD3	2.16	0.45
1:A:54:ASN:HA	1:A:205:ARG:NH1	2.32	0.45
1:A:740:ARG:NH1	1:A:766:ILE:HG22	2.31	0.45
1:A:217:MET:O	1:A:221:MET:HG3	2.17	0.45
1:A:781:LYS:HD2	1:A:782:GLU:N	2.31	0.44
1:A:57:LYS:HZ3	1:A:202:ARG:HG3	1.82	0.44
1:A:240:TYR:HB2	1:A:288:LEU:HD22	1.98	0.44
1:A:738:GLU:HG2	2:B:31:U:O2	2.18	0.44
1:A:809:THR:HG22	1:A:816:PRO:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:H	1:A:68:THR:HG22	1.82	0.44
1:A:65:GLN:HG2	1:A:67:ASN:HD22	1.82	0.44
1:A:84:VAL:HA	1:A:87:THR:HG22	2.00	0.44
1:A:336:VAL:O	1:A:339:ILE:HG12	2.17	0.44
1:A:1018:ASN:HD21	1:A:1036:LEU:HD21	1.83	0.44
1:A:93:GLN:OE1	1:A:95:GLN:N	2.50	0.43
1:A:1016:ARG:HH12	1:A:1043:VAL:HG21	1.81	0.43
1:A:142:PRO:HD2	1:A:148:TYR:CE1	2.53	0.43
1:A:221:MET:HE3	1:A:221:MET:HB3	1.60	0.43
1:A:1019:ILE:HD13	1:A:1036:LEU:HD22	2.00	0.43
1:A:151:GLU:HA	1:A:151:GLU:OE1	2.19	0.43
1:A:423:GLN:HB3	1:A:494:TYR:CZ	2.54	0.43
1:A:687:ILE:HD13	1:A:692:LEU:HB3	2.01	0.43
1:A:821:SER:OG	1:A:908:LEU:O	2.26	0.43
1:A:336:VAL:HG11	1:A:1046:TYR:O	2.18	0.43
1:A:634:ASP:OD1	1:A:634:ASP:N	2.48	0.43
1:A:833:ILE:HG12	1:A:1025:LEU:HA	2.00	0.43
2:B:4:C:H5'	2:B:5:A:H5'	2.01	0.43
1:A:584:ALA:HB1	1:A:698:PRO:HB2	2.00	0.43
1:A:593:LYS:NZ	2:B:32:U:O2	2.52	0.43
1:A:227:LYS:HA	1:A:227:LYS:HD2	1.75	0.42
1:A:515:ILE:HG21	1:A:591:LEU:HB2	2.00	0.42
1:A:539:THR:O	1:A:601:LEU:HB2	2.18	0.42
1:A:825:VAL:HG21	1:A:834:LEU:HD12	2.01	0.42
1:A:1023:ASN:N	1:A:1023:ASN:HD22	2.17	0.42
1:A:416:GLN:NE2	1:A:827:LYS:O	2.52	0.42
2:B:22:A:H4'	2:B:24:C:C5	2.55	0.42
1:A:574:ILE:HD12	1:A:687:ILE:HG21	1.99	0.42
1:A:870:HIS:NE2	2:B:39:G:OP2	2.43	0.42
1:A:1047:ASP:OD1	1:A:1050:LEU:HB2	2.19	0.42
1:A:382:ASN:ND2	1:A:730:LEU:O	2.44	0.42
1:A:420:PHE:HE2	1:A:730:LEU:HA	1.84	0.42
1:A:786:ASP:OD2	1:A:788:GLU:N	2.53	0.42
1:A:126:LEU:HA	1:A:126:LEU:HD23	1.78	0.42
1:A:538:LEU:HD11	1:A:764:GLU:HG2	2.01	0.42
1:A:221:MET:HE1	1:A:942:TYR:HE2	1.85	0.42
1:A:457:LYS:HB2	1:A:457:LYS:HE3	1.66	0.42
1:A:540:SER:HB2	1:A:542:VAL:HG23	2.00	0.42
1:A:787:LYS:HE2	1:A:816:PRO:HG3	2.01	0.42
1:A:57:LYS:NZ	1:A:202:ARG:HH11	2.18	0.42
1:A:373:ILE:HA	1:A:376:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASP:O	1:A:43:ASP:OD2	2.37	0.42
1:A:233:ILE:HG13	1:A:324:GLN:OE1	2.19	0.42
1:A:486:TYR:HB3	1:A:722:ILE:HD12	2.02	0.42
1:A:609:ASP:N	1:A:609:ASP:OD1	2.52	0.42
1:A:279:ILE:HD11	2:B:13:A:C5	2.55	0.42
1:A:686:PHE:CD2	1:A:687:ILE:HG12	2.55	0.42
1:A:1011:ARG:HA	1:A:1011:ARG:HD2	1.80	0.42
1:A:619:LEU:HD23	1:A:619:LEU:HA	1.87	0.41
1:A:38:THR:N	2:B:21:G:OP1	2.48	0.41
1:A:555:GLY:HA3	1:A:575:TYR:CD2	2.55	0.41
1:A:873:TRP:CD2	1:A:1094:LEU:HD23	2.55	0.41
1:A:1034:LEU:HD21	1:A:1083:ILE:HD11	2.02	0.41
1:A:83:VAL:HG22	1:A:189:TYR:HD1	1.85	0.41
1:A:89:CYS:HA	1:A:127:ASN:HB2	2.01	0.41
1:A:49:ILE:HD12	1:A:201:ILE:HD13	2.03	0.41
1:A:206:ILE:HG21	1:A:354:VAL:HG11	2.03	0.41
1:A:893:ILE:HD13	1:A:893:ILE:HA	1.86	0.41
1:A:1056:LYS:HE2	2:B:1:U:O4	2.20	0.41
1:A:322:GLU:O	1:A:326:ILE:HD13	2.19	0.41
1:A:52:ASP:HB2	1:A:54:ASN:O	2.20	0.41
1:A:350:ILE:O	1:A:354:VAL:HG22	2.20	0.41
1:A:1098:SER:OG	1:A:1099:THR:N	2.54	0.41
1:A:152:ILE:HD13	1:A:152:ILE:HA	1.86	0.41
1:A:164:LYS:HB2	1:A:164:LYS:HE2	1.92	0.41
1:A:1069:VAL:HG23	1:A:1083:ILE:HG23	2.03	0.41
1:A:105:GLN:HB2	1:A:108:SER:HB2	2.03	0.41
1:A:150:ILE:HD12	1:A:151:GLU:N	2.27	0.41
1:A:305:ILE:HD13	2:B:18:A:H5'	2.02	0.41
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.87	0.41
1:A:610:LEU:HD12	1:A:610:LEU:HA	1.88	0.41
1:A:826:LYS:HE2	1:A:826:LYS:HB2	1.87	0.41
1:A:928:TYR:HE2	1:A:1054:VAL:HA	1.86	0.41
2:B:4:C:N4	2:B:48:G:O6	2.54	0.40
1:A:38:THR:OG1	2:B:21:G:H5''	2.21	0.40
1:A:142:PRO:HD2	1:A:148:TYR:HE1	1.85	0.40
1:A:444:ILE:O	1:A:448:ILE:HG22	2.22	0.40
1:A:533:PHE:CD1	1:A:603:GLN:HB3	2.56	0.40
1:A:603:GLN:HA	1:A:606:THR:OG1	2.21	0.40
1:A:834:LEU:HD23	1:A:834:LEU:HA	1.90	0.40
1:A:913:HIS:HB3	1:A:1109:TYR:OH	2.22	0.40
1:A:1018:ASN:O	1:A:1023:ASN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:HB2	1:A:91:PRO:HD3	2.03	0.40
1:A:575:TYR:OH	1:A:683:PHE:HB3	2.22	0.40
1:A:1047:ASP:OD2	1:A:1050:LEU:HD12	2.22	0.40
2:B:36:A:N3	2:B:36:A:H2'	2.37	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	900/1120 (80%)	862 (96%)	38 (4%)	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	875/1057 (83%)	767 (88%)	108 (12%)	4	7

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	48	LEU

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Mol	Chain	Res	Type
1	A	57	LYS
1	A	93	GLN
1	A	101	HIS
1	A	144	LYS
1	A	145	SER
1	A	164	LYS
1	A	205	ARG
1	A	246	THR
1	A	272	GLN
1	A	277	GLN
1	A	280	GLU
1	A	286	SER
1	A	299	LEU
1	A	303	PHE
1	A	310	ARG
1	A	332	LYS
1	A	333	ASN
1	A	338	ARG
1	A	342	GLU
1	A	354	VAL
1	A	360	GLN
1	A	371	LYS
1	A	372	PHE
1	A	378	PHE
1	A	388	TYR
1	A	391	CYS
1	A	392	LYS
1	A	408	ILE
1	A	410	HIS
1	A	413	PHE
1	A	423	GLN
1	A	435	TRP
1	A	460	PHE
1	A	465	PHE
1	A	480	VAL
1	A	523	GLN
1	A	536	SER
1	A	551	VAL
1	A	571	LYS
1	A	594	MET
1	A	596	TYR
1	A	608	ASN

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Mol	Chain	Res	Type
1	A	615	VAL
1	A	621	LEU
1	A	632	PHE
1	A	636	ARG
1	A	638	MET
1	A	641	ASP
1	A	658	TYR
1	A	683	PHE
1	A	686	PHE
1	A	697	HIS
1	A	719	ASP
1	A	720	SER
1	A	726	LEU
1	A	729	LYS
1	A	735	GLN
1	A	742	GLU
1	A	743	MET
1	A	747	SER
1	A	748	CYS
1	A	757	SER
1	A	764	GLU
1	A	770	LEU
1	A	771	LEU
1	A	777	CYS
1	A	781	LYS
1	A	786	ASP
1	A	787	LYS
1	A	791	LYS
1	A	793	ASN
1	A	804	GLN
1	A	812	ASP
1	A	815	THR
1	A	820	ARG
1	A	842	ASP
1	A	845	LYS
1	A	849	LYS
1	A	857	TYR
1	A	876	LYS
1	A	881	ARG
1	A	886	THR
1	A	888	LYS
1	A	910	GLN

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Mol	Chain	Res	Type
1	A	912	ARG
1	A	923	SER
1	A	924	ARG
1	A	929	MET
1	A	939	SER
1	A	1012	LEU
1	A	1015	LYS
1	A	1021	HIS
1	A	1023	ASN
1	A	1046	TYR
1	A	1057	SER
1	A	1068	GLU
1	A	1069	VAL
1	A	1070	THR
1	A	1076	GLN
1	A	1082	LYS
1	A	1086	LEU
1	A	1094	LEU
1	A	1097	LYS
1	A	1102	SER
1	A	1105	VAL
1	A	1109	TYR

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

Mol	Chain	Res	Type
1	A	67	ASN
1	A	1023	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	55/65 (84%)	24 (43%)	1 (1%)

All (24) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	A
2	B	4	C
2	B	11	A

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Mol	Chain	Res	Type
2	B	12	U
2	B	13	A
2	B	14	G
2	B	15	U
2	B	16	G
2	B	18	A
2	B	19	G
2	B	20	G
2	B	23	U
2	B	24	C
2	B	25	U
2	B	30	C
2	B	36	A
2	B	38	C
2	B	39	G
2	B	42	G
2	B	46	U
2	B	47	C
2	B	48	G
2	B	49	C
2	B	50	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	37	U

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.