Full wwPDB EM Validation Report ⓘ

Dec 11, 2024 – 04:07 PM JST

PDB ID	:	8JTR
EMDB ID	:	EMD-36650
Title	:	Cryo-EM structure of GeoCas9-sgRNA binary complex
Authors	:	Shen, P.P.; Liu, B.B.; Li, X.; Zhang, L.L.; Chen, C.-C.; Guo, R.-T.
Deposited on	:	2023-06-22
Resolution	:	3.21 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:

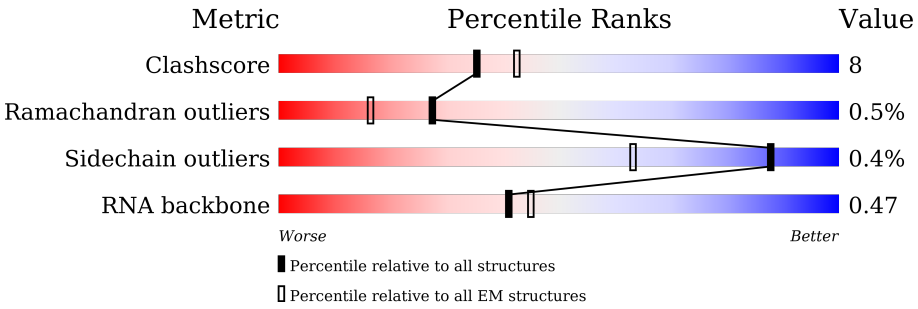
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.21 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 >=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	1095	77% 19% .
2	B	139	34% 28% 14% 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10957 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1056	Total	C	N	O	S	0	0
			8708	5501	1588	1598	21		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	ALA	THR	conflict	UNP A0A150MP45
A	241	ALA	THR	conflict	UNP A0A150MP45
A	353	GLU	GLY	conflict	UNP A0A150MP45
A	582	ALA	HIS	engineered mutation	UNP A0A150MP45
A	1088	LEU	-	expression tag	UNP A0A150MP45
A	1089	GLU	-	expression tag	UNP A0A150MP45
A	1090	HIS	-	expression tag	UNP A0A150MP45
A	1091	HIS	-	expression tag	UNP A0A150MP45
A	1092	HIS	-	expression tag	UNP A0A150MP45
A	1093	HIS	-	expression tag	UNP A0A150MP45
A	1094	HIS	-	expression tag	UNP A0A150MP45
A	1095	HIS	-	expression tag	UNP A0A150MP45

- Molecule 2 is a RNA chain called sgRNA (139-bp).

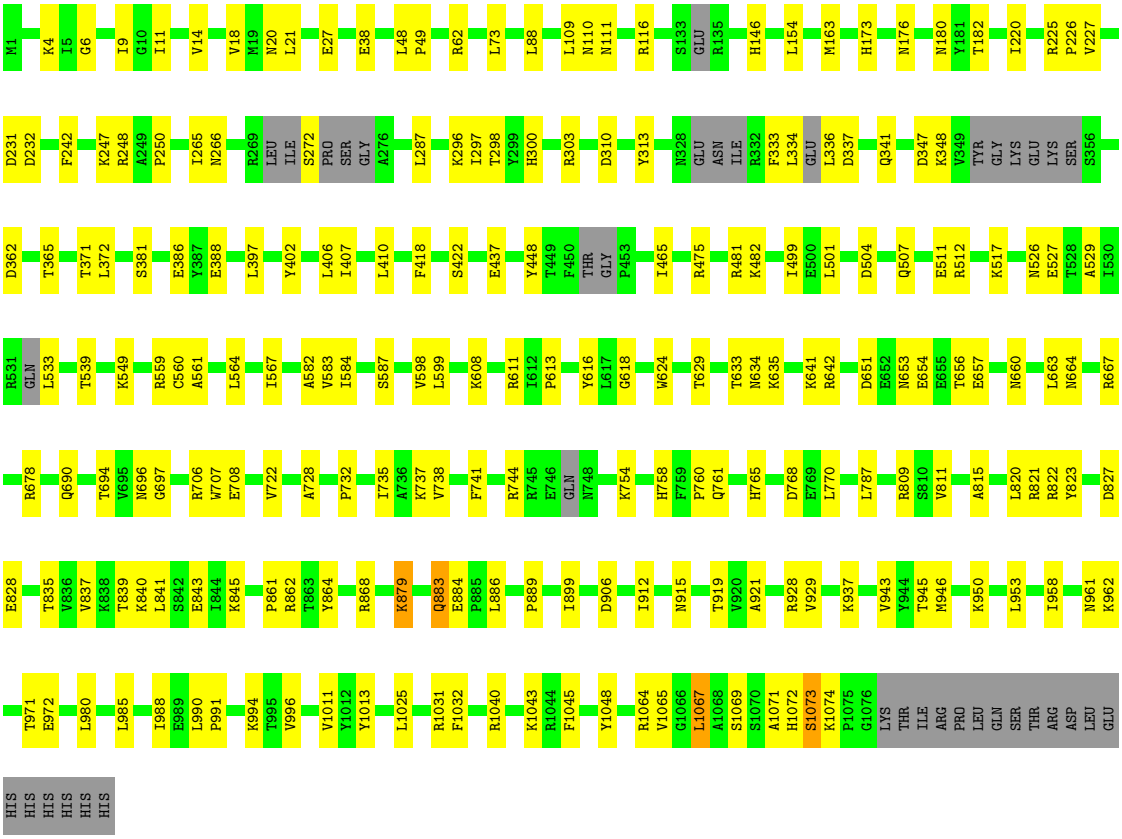
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	105	Total	C	N	O	P	0	0
			2249	1003	409	732	105		

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.

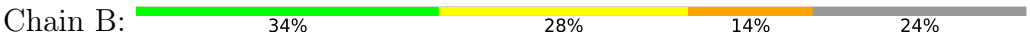
- Molecule 1: CRISPR-associated endonuclease Cas9

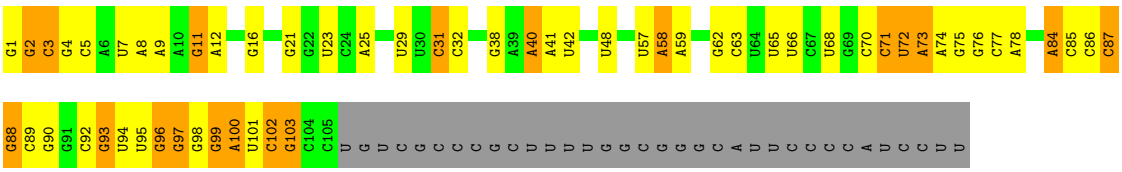
Chain A:



- Molecule 2: sgRNA (139-bp)

Chain B:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	305427	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 ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	1/8876 (0.0%)	0.55	3/11932 (0.0%)
2	B	0.18	0/2516	0.74	0/3922
All	All	0.25	1/11392 (0.0%)	0.61	3/15854 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	732	PRO	CG-CD	-6.78	1.28	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	732	PRO	N-CD-CG	-9.42	89.08	103.20
1	A	732	PRO	CA-N-CD	-7.46	101.05	111.50
1	A	883	GLN	C-N-CA	5.09	134.44	121.70

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	8708	0	8783	145	0
2	B	2249	0	1134	30	0
All	All	10957	0	9917	158	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 8.

All (158) 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:559:ARG:HE	1:A:564:LEU:HD13	1.46	0.80
1:A:1065:VAL:HG12	1:A:1067:LEU:H	1.54	0.73
1:A:928:ARG:NH1	1:A:1065:VAL:O	2.23	0.70
1:A:559:ARG:HH21	1:A:564:LEU:HD22	1.57	0.69
1:A:883:GLN:O	1:A:884:GLU:HG3	1.94	0.68
1:A:958:ILE:O	1:A:1040:ARG:NH2	2.28	0.67
1:A:529:ALA:O	1:A:533:LEU:N	2.28	0.67
1:A:653:ASN:OD1	1:A:654:GLU:N	2.27	0.66
1:A:821:ARG:NH1	1:A:906:ASP:OD2	2.27	0.66
1:A:1074:LYS:HB2	2:B:97:G:H1	1.59	0.66
1:A:225:ARG:NH2	2:B:84:A:O3'	2.29	0.66
1:A:991:PRO:HB3	1:A:1043:LYS:HD2	1.80	0.63
1:A:109:LEU:HG	1:A:110:ASN:H	1.63	0.63
1:A:994:LYS:HG2	1:A:996:VAL:H	1.65	0.62
1:A:613:PRO:HA	1:A:616:TYR:HB3	1.82	0.62
1:A:6:GLY:HA3	1:A:728:ALA:HB2	1.82	0.61
1:A:915:ASN:HD22	1:A:915:ASN:N	1.96	0.61
1:A:388:GLU:OE1	1:A:388:GLU:N	2.34	0.61
1:A:634:ASN:O	1:A:642:ARG:NH2	2.33	0.61
1:A:985:LEU:HD22	1:A:1048:TYR:HB2	1.83	0.60
1:A:38:GLU:OE2	1:A:512:ARG:NH2	2.35	0.60
1:A:641:LYS:HG2	1:A:642:ARG:H	1.67	0.60
2:B:99:G:H4'	2:B:100:A:OP1	2.02	0.60
1:A:110:ASN:OD1	1:A:111:ASN:N	2.35	0.60
1:A:722:VAL:HG22	1:A:770:LEU:HD21	1.83	0.59
1:A:482:LYS:NZ	2:B:92:C:OP1	2.36	0.59
1:A:696:ASN:OD1	1:A:697:GLY:N	2.36	0.59
1:A:971:THR:HG22	1:A:972:GLU:H	1.67	0.59
1:A:1072:HIS:CD2	2:B:99:G:H1	2.20	0.59
1:A:18:VAL:HG23	1:A:27:GLU:HB2	1.84	0.58
1:A:527:GLU:HG3	2:B:2:G:H22	1.69	0.58
1:A:821:ARG:HG2	1:A:837:VAL:HB	1.86	0.58
1:A:953:LEU:HD13	1:A:1064:ARG:HH21	1.67	0.58
2:B:40:A:H4'	2:B:41:A:H5'	1.85	0.58
1:A:303:ARG:NH2	1:A:310:ASP:OD1	2.37	0.57
1:A:465:ILE:HG13	1:A:481:ARG:HD3	1.84	0.57
1:A:988:ILE:HD12	1:A:990:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:THR:HG22	1:A:397:LEU:HB2	1.87	0.56
1:A:402:TYR:HB3	1:A:406:LEU:HD23	1.88	0.56
1:A:475:ARG:NH2	2:B:90:G:H5'	2.22	0.55
1:A:227:VAL:O	2:B:16:G:O2'	2.21	0.55
1:A:402:TYR:HB2	1:A:407:ILE:HD11	1.88	0.55
1:A:929:VAL:HB	1:A:980:LEU:HB2	1.88	0.55
1:A:811:VAL:HG11	1:A:928:ARG:HH21	1.71	0.55
1:A:823:TYR:HA	1:A:835:THR:HG22	1.90	0.54
1:A:499:ILE:HB	1:A:694:THR:HG22	1.88	0.54
1:A:406:LEU:O	1:A:410:LEU:HG	2.08	0.54
1:A:583:VAL:HG12	1:A:584:ILE:HG13	1.89	0.54
1:A:886:LEU:HB2	1:A:899:ILE:HB	1.89	0.54
1:A:707:TRP:HE1	1:A:761:GLN:HE21	1.54	0.54
1:A:765:HIS:CE1	1:A:787:LEU:HD13	2.42	0.54
1:A:1011:VAL:HG21	1:A:1025:LEU:HD13	1.89	0.53
1:A:660:ASN:O	1:A:664:ASN:HB2	2.07	0.53
2:B:71:C:O2	2:B:73:A:O2'	2.25	0.53
1:A:347:ASP:OD1	1:A:348:LYS:N	2.41	0.53
1:A:582:ALA:HB2	1:A:598:VAL:H	1.73	0.53
1:A:9:ILE:HD13	1:A:14:VAL:HG23	1.91	0.52
1:A:629:THR:O	1:A:633:THR:HG23	2.10	0.52
1:A:678:ARG:HH12	1:A:690:GLN:HG3	1.74	0.52
1:A:11:ILE:HD11	1:A:504:ASP:HB2	1.92	0.52
2:B:2:G:H4'	2:B:3:C:OP2	2.10	0.52
1:A:526:ASN:ND2	2:B:3:C:OP1	2.43	0.51
2:B:57:U:H5"	2:B:58:A:H4'	1.93	0.51
1:A:482:LYS:HZ1	2:B:92:C:P	2.35	0.50
1:A:839:THR:OG1	1:A:843:GLU:OE2	2.30	0.50
2:B:31:C:H42	2:B:48:U:H3	1.60	0.50
1:A:146:HIS:CD2	1:A:182:THR:HA	2.48	0.49
1:A:845:LYS:HE3	1:A:879:LYS:HB3	1.95	0.49
2:B:87:C:O2'	2:B:88:G:OP1	2.29	0.49
1:A:827:ASP:OD1	1:A:828:GLU:N	2.46	0.49
1:A:560:CYS:HB3	1:A:567:ILE:HG13	1.94	0.49
1:A:225:ARG:HD3	1:A:226:PRO:HD2	1.94	0.48
1:A:706:ARG:HH11	2:B:1:G:N2	2.10	0.48
1:A:656:THR:O	1:A:660:ASN:ND2	2.46	0.48
1:A:1072:HIS:O	1:A:1073:SER:HB3	2.13	0.48
1:A:937:LYS:HE3	1:A:1040:ARG:HB3	1.94	0.48
1:A:635:LYS:HD2	1:A:635:LYS:HA	1.68	0.48
1:A:915:ASN:N	1:A:915:ASN:ND2	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:SER:N	1:A:313:TYR:O	2.46	0.48
1:A:154:LEU:HD22	1:A:163:MET:SD	2.55	0.47
1:A:657:GLU:HA	1:A:660:ASN:HD21	1.80	0.47
1:A:651:ASP:N	1:A:651:ASP:OD1	2.45	0.47
1:A:1072:HIS:HE1	2:B:93:G:H1	1.63	0.47
1:A:73:LEU:HD22	1:A:220:ILE:HD12	1.96	0.47
1:A:507:GLN:O	1:A:511:GLU:HB2	2.15	0.47
1:A:608:LYS:O	1:A:611:ARG:NH1	2.48	0.47
1:A:741:PHE:HA	1:A:744:ARG:HG2	1.97	0.47
1:A:864:TYR:CG	1:A:868:ARG:HG2	2.49	0.47
1:A:912:ILE:N	1:A:921:ALA:O	2.37	0.47
1:A:707:TRP:O	1:A:708:GLU:HG2	2.15	0.47
1:A:815:ALA:HA	1:A:945:THR:HB	1.97	0.46
1:A:560:CYS:SG	1:A:561:ALA:N	2.86	0.46
1:A:861:PRO:O	1:A:862:ARG:NH1	2.47	0.46
1:A:298:THR:HG22	1:A:300:HIS:H	1.81	0.46
1:A:1031:ARG:HG3	1:A:1032:PHE:CD2	2.50	0.46
1:A:88:LEU:HD21	1:A:116:ARG:HG3	1.97	0.45
1:A:828:GLU:N	1:A:828:GLU:OE1	2.46	0.45
2:B:96:G:O2'	2:B:97:G:H2'	2.16	0.45
1:A:173:HIS:CE1	1:A:176:ASN:HA	2.51	0.45
2:B:72:U:O2'	2:B:73:A:O2'	2.34	0.45
2:B:58:A:O2'	2:B:59:A:H8	1.99	0.45
2:B:68:U:H3	2:B:78:A:H61	1.64	0.45
1:A:475:ARG:HH21	2:B:90:G:H5'	1.81	0.45
1:A:953:LEU:HD23	1:A:953:LEU:HA	1.82	0.44
2:B:102:C:H1'	2:B:103:G:C8	2.52	0.44
1:A:20:ASN:OD1	1:A:21:LEU:N	2.50	0.44
1:A:504:ASP:N	1:A:504:ASP:OD1	2.50	0.44
1:A:663:LEU:HD11	1:A:735:ILE:HD13	1.98	0.44
1:A:765:HIS:NE2	1:A:787:LEU:HD13	2.31	0.44
1:A:62:ARG:HH12	1:A:225:ARG:NH2	2.15	0.44
1:A:247:LYS:HB3	1:A:247:LYS:HE3	1.84	0.44
1:A:265:ILE:HG23	1:A:287:LEU:HD23	2.00	0.44
1:A:618:GLY:C	1:A:624:TRP:HE1	2.20	0.44
1:A:822:ARG:HD3	2:B:25:A:OP1	2.17	0.44
1:A:737:LYS:NZ	1:A:760:PRO:HG2	2.33	0.44
1:A:758:HIS:CD2	2:B:1:G:H1	2.36	0.44
1:A:840:LYS:HG3	1:A:841:LEU:H	1.83	0.44
1:A:928:ARG:HG2	1:A:943:VAL:HB	2.00	0.44
1:A:641:LYS:CG	1:A:642:ARG:H	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:ILE:HG23	1:A:735:ILE:O	2.18	0.44
1:A:980:LEU:HD21	1:A:1045:PHE:HZ	1.83	0.44
1:A:297:ILE:O	1:A:333:PHE:N	2.50	0.43
1:A:737:LYS:HA	1:A:737:LYS:HE3	2.00	0.43
1:A:862:ARG:HD2	1:A:889:PRO:O	2.18	0.43
1:A:231:ASP:OD1	1:A:232:ASP:N	2.52	0.43
1:A:242:PHE:HD2	1:A:448:TYR:HD1	1.65	0.43
1:A:334:LEU:HB3	1:A:336:LEU:HD22	2.01	0.43
1:A:811:VAL:O	1:A:811:VAL:HG23	2.19	0.43
1:A:1072:HIS:CE1	2:B:93:G:H1	2.35	0.43
2:B:11:G:H2'	2:B:12:A:C8	2.53	0.43
1:A:946:MET:HG3	1:A:950:LYS:HE2	2.01	0.43
1:A:501:LEU:O	1:A:667:ARG:NH2	2.43	0.43
1:A:868:ARG:HD3	1:A:868:ARG:HA	1.85	0.42
1:A:517:LYS:HB3	1:A:517:LYS:HE2	1.86	0.42
1:A:915:ASN:HD22	1:A:915:ASN:H	1.66	0.42
1:A:820:LEU:O	2:B:23:U:O2'	2.34	0.42
1:A:250:PRO:HB3	1:A:371:THR:HG21	2.00	0.42
1:A:180:ASN:HB3	1:A:182:THR:HG23	2.02	0.42
1:A:266:ASN:ND2	1:A:437:GLU:O	2.53	0.42
1:A:587:SER:HA	1:A:738:VAL:HG12	2.02	0.41
1:A:815:ALA:H	2:B:58:A:H62	1.68	0.41
1:A:961:ASN:O	1:A:962:LYS:HD3	2.19	0.41
1:A:337:ASP:O	1:A:341:GLN:HG3	2.19	0.41
1:A:362:ASP:O	1:A:365:THR:OG1	2.29	0.41
1:A:980:LEU:HD23	1:A:1013:TYR:CD1	2.55	0.41
1:A:862:ARG:HD3	1:A:862:ARG:HA	1.90	0.41
1:A:583:VAL:HG22	1:A:613:PRO:HG2	2.01	0.41
1:A:549:LYS:HD2	1:A:599:LEU:HD13	2.03	0.41
1:A:372:LEU:HD21	1:A:418:PHE:HZ	1.85	0.41
1:A:608:LYS:HE2	1:A:613:PRO:HG3	2.03	0.41
1:A:48:LEU:HB3	1:A:49:PRO:HD3	2.03	0.41
1:A:248:ARG:HA	1:A:422:SER:HA	2.02	0.41
1:A:937:LYS:HE2	1:A:1040:ARG:HD2	2.02	0.41
1:A:381:SER:HB2	1:A:386:GLU:HB2	2.03	0.40
1:A:820:LEU:HD13	1:A:919:THR:HG21	2.04	0.40
1:A:4:LYS:HE2	1:A:21:LEU:HD21	2.04	0.40
1:A:371:THR:HG23	1:A:372:LEU:HG	2.03	0.40
1:A:765:HIS:HB2	1:A:768:ASP:HB3	2.03	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	1037/1095 (95%)	951 (92%)	81 (8%)	5 (0%)	25 59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1069	SER
1	A	1071	ALA
1	A	1073	SER
1	A	1067	LEU
1	A	539	THR

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	947/983 (96%)	943 (100%)	4 (0%)	89 93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	LYS
1	A	754	LYS
1	A	809	ARG
1	A	879	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	522	ASN
1	A	660	ASN
1	A	1072	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	104/139 (74%)	43 (41%)	7 (6%)

All (43) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	G
2	B	3	C
2	B	4	G
2	B	5	C
2	B	7	U
2	B	8	A
2	B	9	A
2	B	11	G
2	B	21	G
2	B	29	U
2	B	31	C
2	B	32	C
2	B	38	G
2	B	40	A
2	B	42	U
2	B	58	A
2	B	62	G
2	B	63	C
2	B	66	U
2	B	70	C
2	B	71	C
2	B	72	U
2	B	73	A
2	B	74	A
2	B	75	G
2	B	76	G
2	B	77	C
2	B	84	A
2	B	85	C
2	B	86	C

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Mol	Chain	Res	Type
2	B	88	G
2	B	89	C
2	B	93	G
2	B	94	U
2	B	95	U
2	B	96	G
2	B	97	G
2	B	98	G
2	B	99	G
2	B	100	A
2	B	101	U
2	B	102	C
2	B	103	G

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	2	G
2	B	65	U
2	B	84	A
2	B	87	C
2	B	98	G
2	B	99	G
2	B	100	A

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.