wwPDB X-ray Structure Validation Summary Report (i)

Jun 3, 2024 – 02:53 PM JST

PDB ID	:	8KAI
Title	:	Crystal structure of SpyCas9-crRNA-tracrRNA complex bound to 17nt target DNA
Authors	:	Chen, Y.; Chen, J.; Liu, L.
Deposited on	:	2023-08-03
Resolution	:	3.49 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

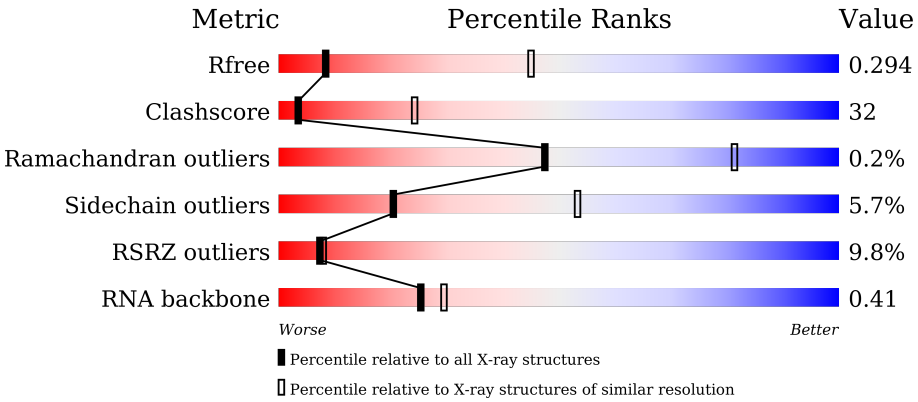
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	34	6% 9% 38% 32% 21%
1	E	34	9% 24% 26% 38% • 9%
2	B	1368	9% 45% 48% • •
2	F	1368	11% 44% 48% 5% •

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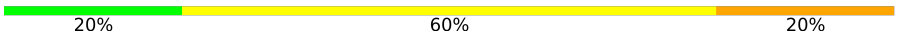
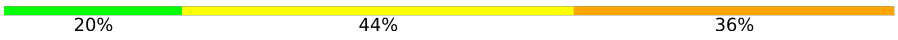
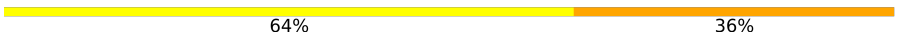
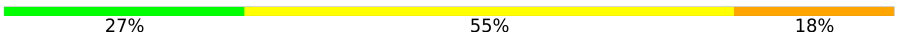
Mol	Chain	Length	Quality of chain
3	C	25	
3	G	25	
4	D	11	
4	H	11	
5	I	65	
5	J	65	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 27007 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	34	Total	C	N	O	P	0	0	0
			725	325	127	239	34			
1	E	31	Total	C	N	O	P	0	0	0
			663	297	118	217	31			

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1326	Total	C	N	O	S	0	0	0
			10769	6854	1869	2024	22			
2	F	1327	Total	C	N	O	S	0	0	0
			10698	6816	1845	2014	23			

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	25	Total	C	N	O	P	0	0	0
			501	244	83	150	24			
3	G	25	Total	C	N	O	P	0	0	0
			501	244	83	150	24			

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			225	110	37	68	10			
4	H	11	Total	C	N	O	P	0	0	0
			225	110	37	68	10			

- Molecule 5 is a RNA chain called RNA (65-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	63	Total	C	N	O	P	0	0	0
			1348	603	245	437	63			
5	J	63	Total	C	N	O	P	0	0	0
			1348	603	245	437	63			

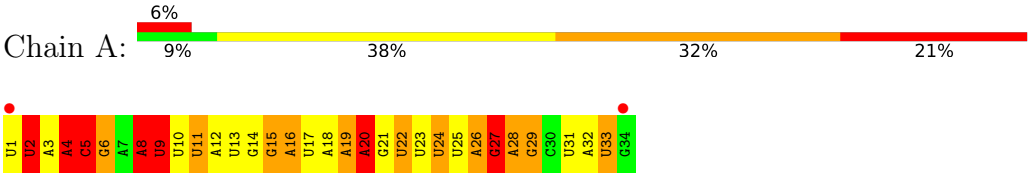
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	O	0	0
			1	1		
6	F	3	Total	O	0	0
			3	3		

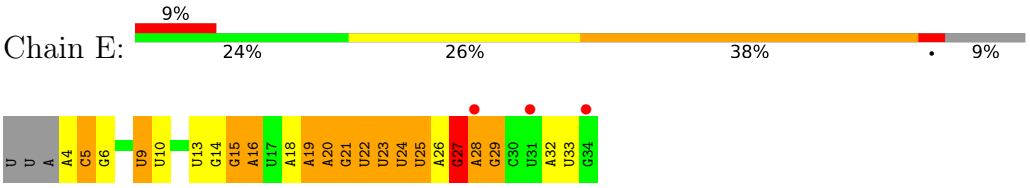
3 Residue-property plots (i)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

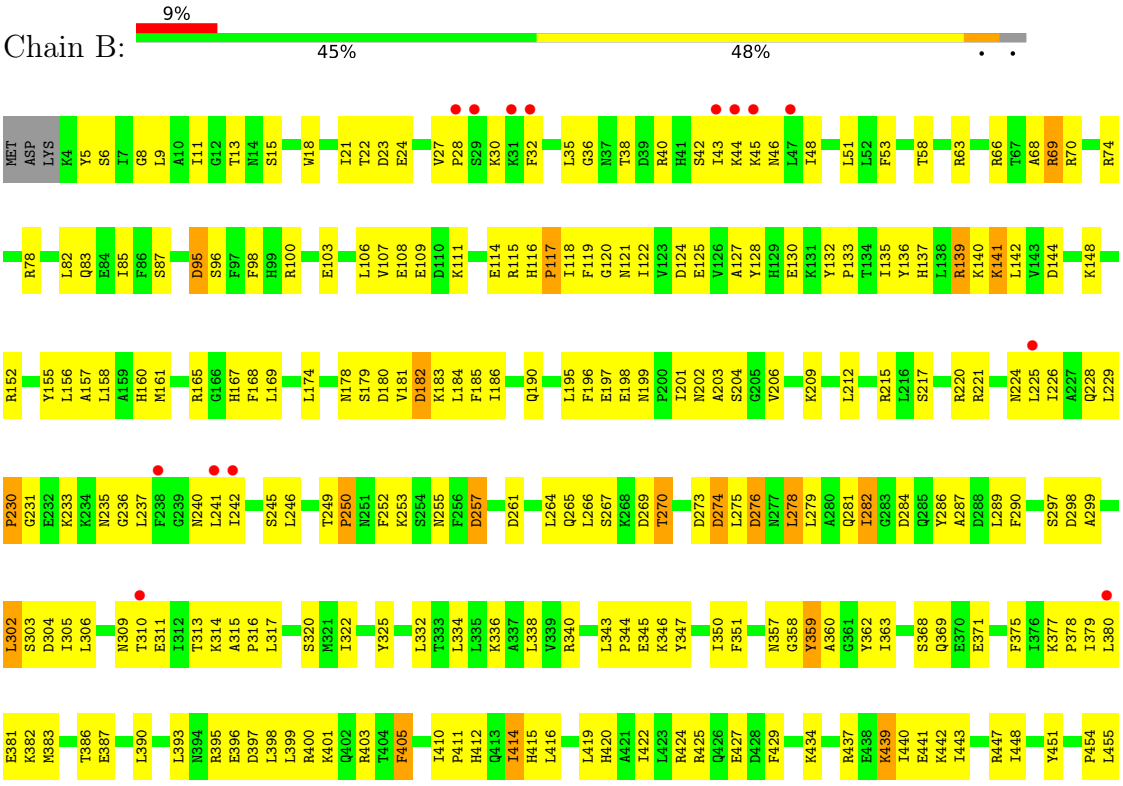
• Molecule 1: RNA (34-MER)

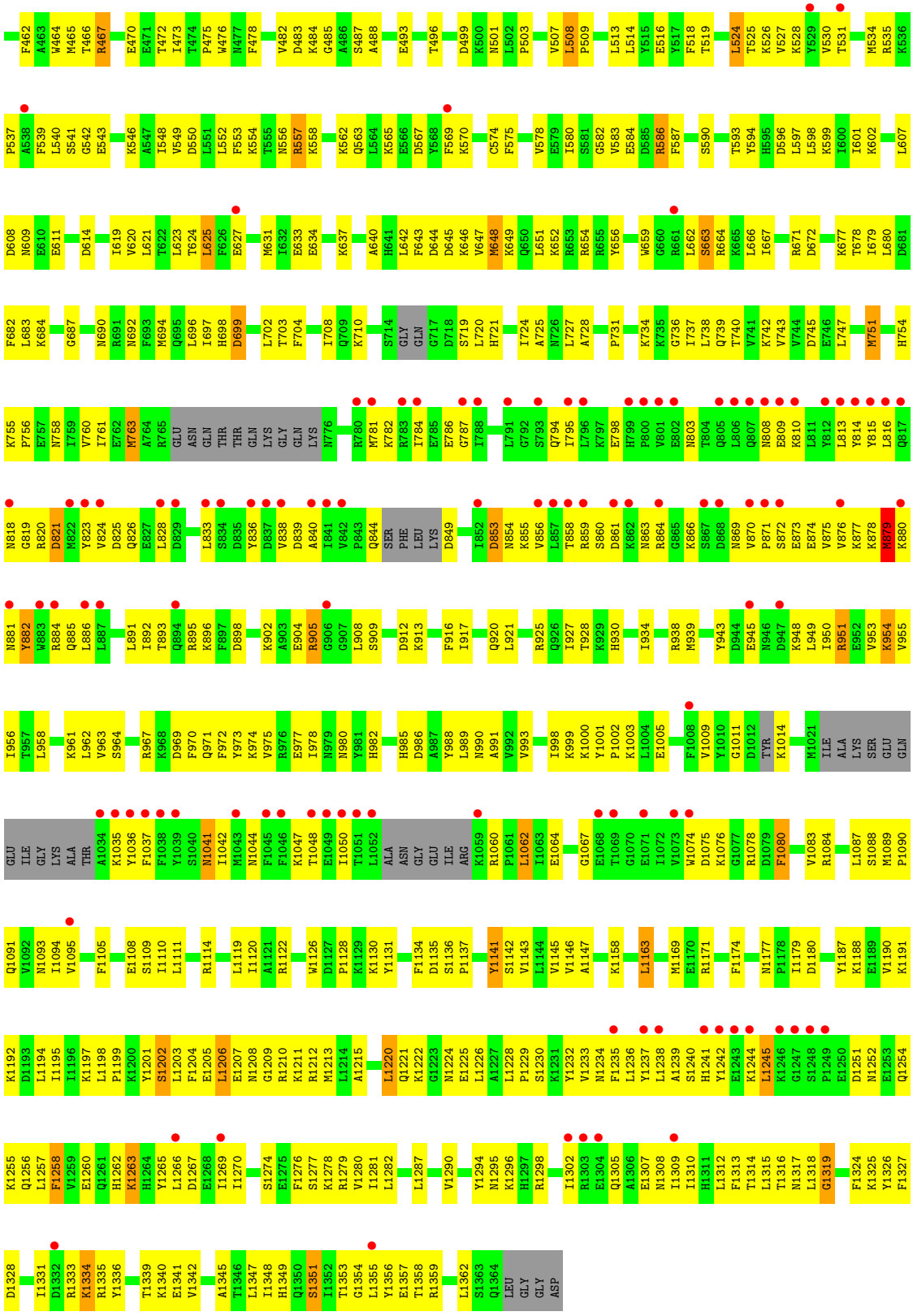


• Molecule 1: RNA (34-MER)



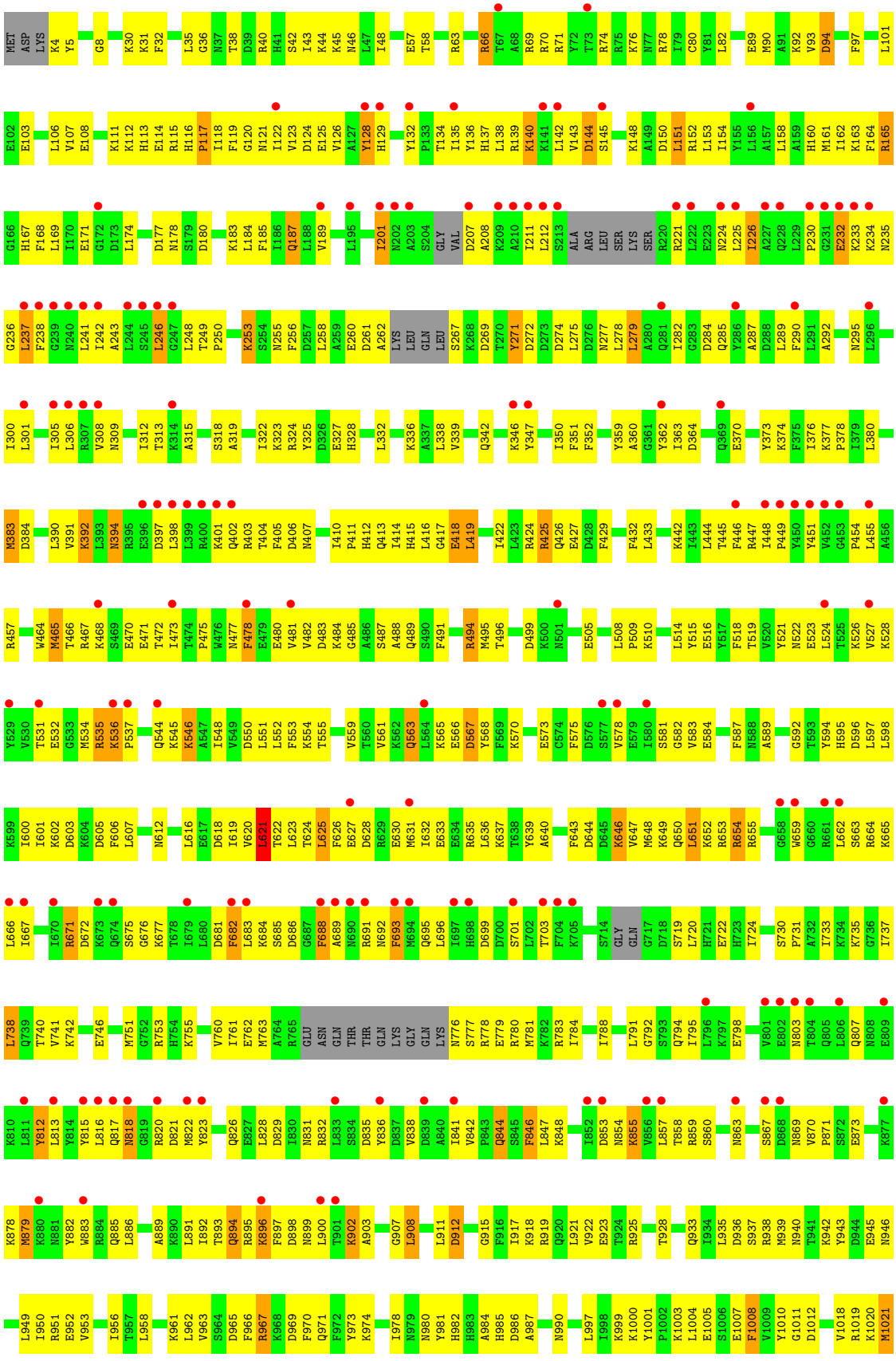
• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

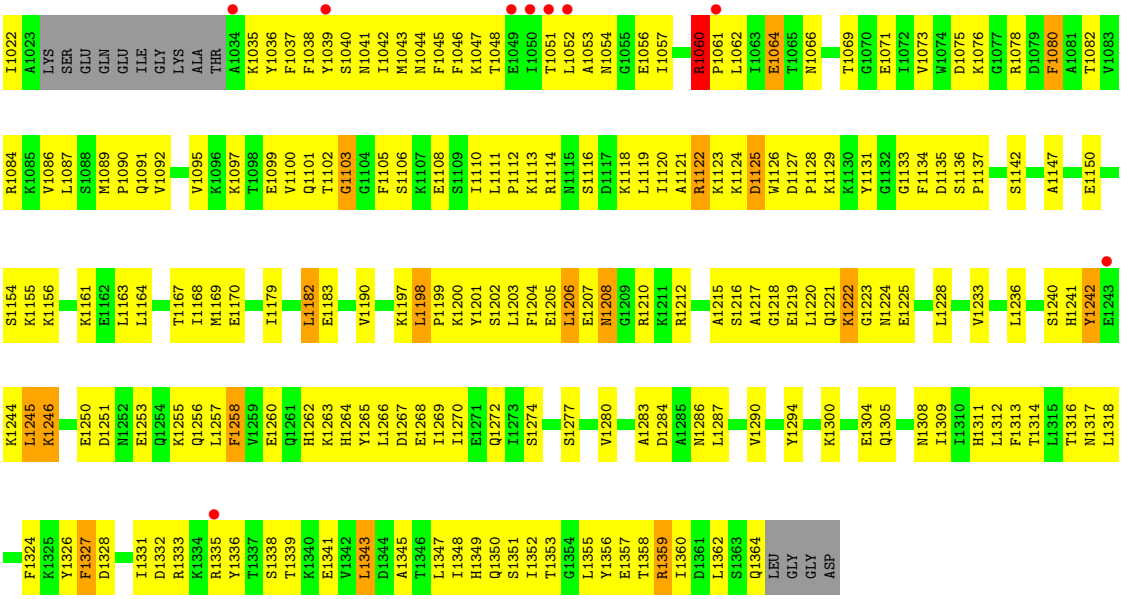




• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

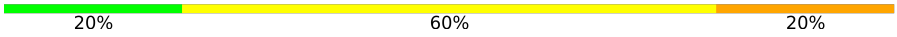
Chain F:


MET ASP LYS K4 Y5 G8 K30 K31 F32 L35 G36 N37 T38 D39 R40 H41 S42 I43 K44 K45 N46 L47 I48 E57 T58 R63 R66 T67 A68 R69 R70 R71 Y72 T73 R74 R75 K76 N77 R78 I79 C80 Y81 L82 E89 M90 A91 K92 V93 D94 F97 L101
E102 E103 L106 V107 E108 K111 K112 H113 E114 R115 H116 P117 I118 F119 G120 N121 I122 V123 D124 E125 V126 A127 Y128 H129 Y132 P133 T134 I135 Y136 H137 L138 R139 K140 K141 L142 V143 D144 S145 K148 A149 D150 L151 R152 L153 I154 Y155 L156 A157 L158 A159 H160 M161 I162 K163 F164 R165
G166 H167 F168 L169 I170 E171 G172 D173 L174 D177 N178 S179 D180 K183 L184 F185 I186 Q187 L188 V189 L195 I201 N202 A203 S204 GLY VAL D207 A208 K209 A210 I211 L212 S213 ALA ARG LEU SER LYS SER R220 R221 L222 E223 N224 L225 I226 A227 Q228 L229 P230 G231 E232 K233 K234 N235
G236 L237 F238 G239 N240 L241 I242 A243 L244 S245 L246 G247 L248 T249 P250 K253 S254 N255 F256 D257 L258 A259 E260 D261 A262 LYS LEU GLN LEU S267 K268 D269 T270 Y271 D272 D273 D274 L275 D276 N277 L278 L279 A280 Q281 I282 G283 D284 Q285 Y286 A287 D288 L289 F290 L291 A292 N295 L296
I300 L301 I305 L306 R307 V308 N309 I312 T313 K314 A315 S318 A319 I322 K323 R324 Y325 D326 E327 H328 L332 K336 A337 L338 V339 Q342 K346 Y347 I350 F351 F352 Y359 A360 G361 Y362 I363 D364 Q369 E370 Y373 K374 F375 I376 K377 P378 I379 L380
M383 D384 L390 V391 K392 L393 N394 R395 E396 D397 L398 L399 R400 K401 Q402 R403 T404 F405 D406 N407 I410 P411 H412 Q413 I414 H415 L416 G417 E418 L419 T422 L423 R424 R425 Q426 E427 D428 F429 F432 L433 K442 T443 L444 T445 F446 R447 I448 P449 Y450 Y451 V452 G453 P454 L455 A456
R457 W464 M465 T466 R467 K468 S469 E470 E471 T472 I473 T474 P475 W476 N477 F478 E479 E480 V481 V482 D483 K484 G485 A486 S487 A488 Q489 S490 F491 R494 M495 T496 D499 K500 N501 E505 L508 P509 K510 L514 Y515 E516 Y517 F518 T519 V520 Y521 N522 E523 L524 T525 K526 V527 K528
Y529 V530 T531 E532 G533 M534 R535 K536 P537 Q544 K545 K546 A547 I548 V549 D550 L551 L552 F553 K554 T555 V559 T560 V561 K562 Q563 L564 K565 E566 D567 Y568 F569 K570 E573 C574 F575 D576 S577 V578 E579 I580 S581 G582 V583 E584 F587 N588 A589 G592 T593 Y594 H595 D596 L597 L598
K599 I600 I601 K602 D603 K604 D605 F606 L607 N612 L616 E617 D618 I619 V620 L621 T622 L623 T624 L625 F626 E627 D628 R629 E630 M631 I632 E633 E634 R635 L636 K637 T638 Y639 A640 F643 D644 D645 K646 V647 M648 K649 Q650 L651 K652 R653 R654 R655 G658 W659 G660 R661 L662 S663 R664 K665
L666 I667 I670 R671 D672 K673 Q674 S675 G676 K677 T678 I679 L680 D681 F682 L683 K684 S685 D686 G687 F688 A689 F626 N690 R691 N692 F693 M694 Q695 L696 I697 H698 D699 D700 S701 L702 T703 F704 K705 S714 GLY GLN G717 D718 S719 L720 H721 E722 H723 I724 S730 P731 A732 I733 K734 K735 G736 I737
L738 Q739 T740 V741 K742 E746 M751 G752 R753 H754 K755 V760 I761 E762 M763 A764 R765 GLU ASN GLN THR THR GLN LYS GLY GLN LYS N776 S777 R778 E779 R780 M781 K782 R783 I784 I788 L791 G792 S793 Q794 I795 L796 K797 E798 V801 E802 N803 T804 Q805 L806 Q807 N808 E809
K810 L811 Y812 L813 Y814 Y815 L816 Q817 N818 G819 R820 D821 M822 Y823 Q826 E827 L828 D829 I830 N831 R832 L833 S834 D835 Y836 D837 V838 D839 A840 I841 V842 P843 Q844 S845 F846 L847 K848 I852 D853 N854 K855 V856 L857 T858 R859 S860 N863 S867 D868 N869 V870 P871 S872 E873 K877
K878 M879 K880 N881 Y882 W883 R884 Q885 L886 A889 K890 L891 I892 T893 Q894 R895 K896 F897 D898 N899 L900 T901 K902 A903 G907 L908 L911 D912 G915 F916 I917 K918 R919 Q920 L921 V922 E923 T924 R925 T928 Q933 I934 L935 D936 S937 R938 M939 N940 T941 K942 Y943 D944 E945 N946
L949 I950 R951 E952 V953 I956 T957 L958 K961 L962 V963 S964 D965 F966 R967 K968 D969 F970 Q971 F972 Y973 K974 I978 N979 N980 Y981 H982 H983 A984 H985 D986 A987 N990 L997 I998 K999 K1000 Y1001 P1002 K1003 L1004 E1005 S1006 E1007 F1008 V1009 Y1010 G1011 D1012 V1018 R1019 K1020 M1021



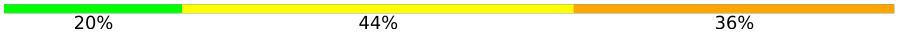
• Molecule 3: DNA (25-MER)

Chain C:



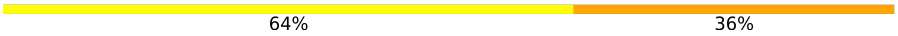
• Molecule 3: DNA (25-MER)

Chain G:



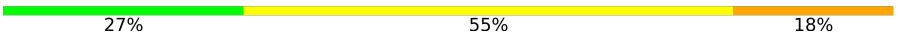
• Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')

Chain D:



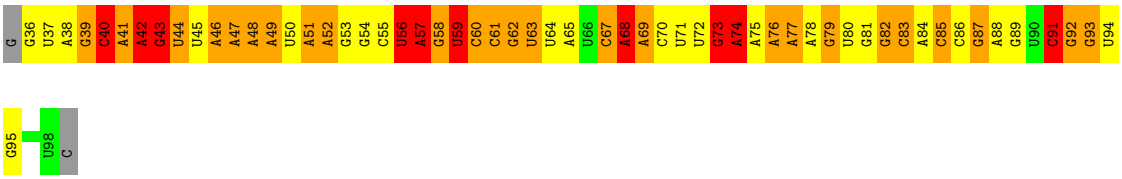
• Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')

Chain H:



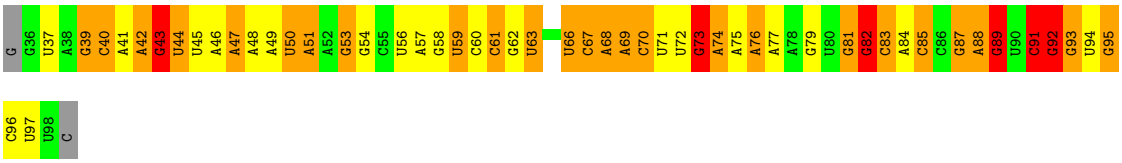
• Molecule 5: RNA (65-MER)

Chain I:



• Molecule 5: RNA (65-MER)

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	144.30Å 130.19Å 146.41Å 90.00° 104.02° 90.00°	Depositor
Resolution (Å)	48.57 – 3.49 48.57 – 3.45	Depositor EDS
% Data completeness (in resolution range)	79.0 (48.57-3.49) 76.2 (48.57-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.225 , 0.294 0.225 , 0.294	Depositor DCC
R_{free} test set	2620 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	62.1	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.087 for l,-k,h	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	27007	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	1.18	2/811 (0.2%)	2.15	52/1261 (4.1%)
1	E	1.03	1/742 (0.1%)	1.89	24/1154 (2.1%)
2	B	0.68	5/10954 (0.0%)	0.89	26/14725 (0.2%)
2	F	0.69	7/10882 (0.1%)	0.90	23/14639 (0.2%)
3	C	1.69	8/559 (1.4%)	1.64	14/859 (1.6%)
3	G	1.60	8/559 (1.4%)	1.53	12/859 (1.4%)
4	D	1.81	4/251 (1.6%)	1.44	2/387 (0.5%)
4	H	1.56	1/251 (0.4%)	1.57	4/387 (1.0%)
5	I	1.19	3/1509 (0.2%)	2.11	93/2350 (4.0%)
5	J	1.09	2/1509 (0.1%)	1.98	66/2350 (2.8%)
All	All	0.85	41/28027 (0.1%)	1.23	316/38971 (0.8%)

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	16	DA	C3'-O3'	-9.28	1.31	1.44
5	I	47	A	C6-N1	-8.44	1.29	1.35
4	D	3	DT	C3'-O3'	-8.17	1.33	1.44
3	G	1	DC	C3'-O3'	8.03	1.54	1.44
2	F	425	ARG	CG-CD	-7.73	1.32	1.51

The worst 5 of 316 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	59	U	O5'-P-OP2	-14.53	92.62	105.70
5	J	91	C	C5-C4-N4	-13.11	111.02	120.20
5	I	48	A	C8-N9-C4	12.70	110.88	105.80
5	I	62	G	C5-C6-O6	12.51	136.11	128.60
5	J	91	C	C5-C6-N1	10.97	126.48	121.00

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	725	0	362	29	0
1	E	663	0	331	30	0
2	B	10769	0	10863	701	2
2	F	10698	0	10745	807	0
3	C	501	0	287	13	0
3	G	501	0	287	19	0
4	D	225	0	129	7	0
4	H	225	0	129	11	0
5	I	1348	0	678	70	0
5	J	1348	0	678	68	0
6	B	1	0	0	0	0
6	F	3	0	0	0	0
All	All	27007	0	24489	1634	2

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 32.

The worst 5 of 1634 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:B:380:LEU:O	2:B:386:THR:CG2	1.70	1.39
2:B:1222:LYS:NZ	2:B:1315:LEU:O	1.59	1.33
2:F:878:LYS:HB3	2:F:879:MET:SD	1.74	1.28
2:F:878:LYS:HD2	2:F:879:MET:CE	1.76	1.16
2:B:410:ILE:HG23	2:B:414:ILE:HD11	1.26	1.15

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:ASN:OD1	2:B:541:SER:OG[2_545]	2.07	0.13
2:B:228:GLN:NE2	2:B:543:GLU:OE2[2_545]	2.18	0.02

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 X-ray entries followed by that with respect to entries of similar resolution.

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
2	B	1312/1368 (96%)	1279 (98%)	29 (2%)	4 (0%)	41 75
2	F	1313/1368 (96%)	1266 (96%)	45 (3%)	2 (0%)	47 81
All	All	2625/2736 (96%)	2545 (97%)	74 (3%)	6 (0%)	47 81

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	270	THR
2	F	1020	LYS
2	F	117	PRO
2	B	117	PRO
2	B	250	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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
2	B	1173/1225 (96%)	1114 (95%)	59 (5%)	24 58
2	F	1156/1225 (94%)	1083 (94%)	73 (6%)	18 51
All	All	2329/2450 (95%)	2197 (94%)	132 (6%)	20 53

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	1080	PHE

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Mol	Chain	Res	Type
2	F	1202	SER
2	F	1338	SER
2	B	1202	SER
2	B	1171	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1364	GLN
2	F	329	HIS
2	F	1256	GLN
2	F	187	GLN
2	F	415	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	33/34 (97%)	9 (27%)	3 (9%)
1	E	30/34 (88%)	9 (30%)	1 (3%)
5	I	62/65 (95%)	20 (32%)	2 (3%)
5	J	62/65 (95%)	19 (30%)	1 (1%)
All	All	187/198 (94%)	57 (30%)	7 (3%)

5 of 57 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	4	A
1	A	5	C
1	A	6	G
1	A	9	U

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	27	G
5	I	42	A
5	J	42	A
5	I	68	A
1	A	28	A

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)

There are no ligands in this entry.

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	34/34 (100%)	0.17	2 (5%) 22 20	19, 34, 129, 166	0
1	E	31/34 (91%)	0.32	3 (9%) 7 8	40, 71, 175, 230	0
2	B	1326/1368 (96%)	0.36	125 (9%) 8 9	13, 62, 175, 215	0
2	F	1327/1368 (97%)	0.46	157 (11%) 4 5	11, 88, 145, 197	0
3	C	25/25 (100%)	-0.31	0 100 100	25, 38, 81, 88	0
3	G	25/25 (100%)	-0.11	0 100 100	45, 59, 118, 139	0
4	D	11/11 (100%)	-0.11	0 100 100	30, 38, 122, 159	0
4	H	11/11 (100%)	-0.21	0 100 100	33, 60, 119, 189	0
5	I	63/65 (96%)	-0.26	0 100 100	17, 71, 122, 170	0
5	J	63/65 (96%)	-0.37	0 100 100	26, 58, 137, 191	0
All	All	2916/3006 (97%)	0.36	287 (9%) 7 8	11, 70, 162, 230	0

The worst 5 of 287 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	801	VAL	23.0
2	B	809	GLU	18.3
2	F	232	GLU	15.7
2	F	231	GLY	12.1
2	B	810	LYS	11.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.