



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2021 – 12:14 PM JST

PDB ID : 7EI1
Title : Structure of Pyrococcus furiosus Cas1Cas2 complex
Authors : Yu, Y.; Chen, Q.
Deposited on : 2021-03-30
Resolution : 3.90 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

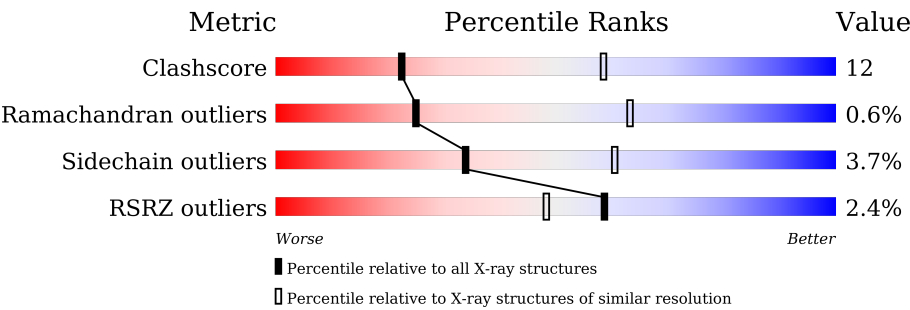
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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))
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 $\leq 5\%$. 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	322	<div><div>4%</div><div><div></div><div>73%</div><div>21%</div><div>..</div></div></div>
1	B	322	<div><div>%</div><div><div></div><div>65%</div><div>30%</div><div>..</div></div></div>
1	C	322	<div><div>3%</div><div><div></div><div>63%</div><div>31%</div><div>..</div></div></div>
1	D	322	<div><div></div><div><div></div><div>63%</div><div>29%</div><div>...</div></div></div>
1	E	322	<div><div>2%</div><div><div></div><div>69%</div><div>26%</div><div>..</div></div></div>
1	F	322	<div><div>3%</div><div><div></div><div>70%</div><div>25%</div><div>..</div></div></div>
1	G	322	<div><div>2%</div><div><div></div><div>70%</div><div>25%</div><div>..</div></div></div>

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Mol	Chain	Length	Quality of chain
1	H	322	 3% 77% 17% 5%
1	I	322	 2% 70% 23% 5%
1	J	322	 2% 78% 16% 5%
1	K	322	 1% 68% 26% 5%
1	L	322	 1% 68% 26% 5%
1	M	322	 4% 65% 30% 5%
1	N	322	 4% 76% 18% 5%
1	O	322	 3% 71% 24% 5%
1	P	322	 4% 75% 18% 5%
2	Q	85	 2% 84% 15% 5%
2	R	85	 4% 89% 9% 5%
2	S	85	 2% 80% 18% 5%
2	T	85	 0% 82% 16% 5%
2	U	85	 2% 73% 26% 5%
2	V	85	 0% 73% 22% 5%
2	W	85	 2% 78% 20% 5%
2	X	85	 1% 85% 14% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 90949 atoms, of which 44675 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 protein called CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	311	Total 5002	C 1647	H 2443	N 449	O 458	S 5	0	0	0
1	B	308	Total 4941	C 1633	H 2409	N 439	O 455	S 5	0	0	0
1	C	312	Total 5020	C 1656	H 2450	N 450	O 459	S 5	0	0	0
1	D	308	Total 4937	C 1633	H 2405	N 439	O 455	S 5	0	0	0
1	E	312	Total 5003	C 1656	H 2433	N 450	O 459	S 5	0	0	0
1	F	308	Total 4950	C 1633	H 2418	N 439	O 455	S 5	0	0	0
1	G	312	Total 5016	C 1656	H 2446	N 450	O 459	S 5	0	0	0
1	H	306	Total 4926	C 1624	H 2408	N 437	O 452	S 5	0	0	0
1	K	310	Total 5012	C 1636	H 2467	N 447	O 457	S 5	0	0	0
1	L	308	Total 4958	C 1633	H 2426	N 439	O 455	S 5	0	0	0
1	M	314	Total 5070	C 1668	H 2481	N 455	O 461	S 5	0	0	0
1	N	305	Total 4905	C 1619	H 2396	N 436	O 449	S 5	0	0	0
1	I	312	Total 5037	C 1656	H 2467	N 450	O 459	S 5	0	0	0
1	J	307	Total 4924	C 1629	H 2399	N 438	O 453	S 5	0	0	0
1	O	311	Total 5024	C 1647	H 2465	N 449	O 458	S 5	0	0	0
1	P	306	Total 4937	C 1624	H 2419	N 437	O 452	S 5	0	0	0

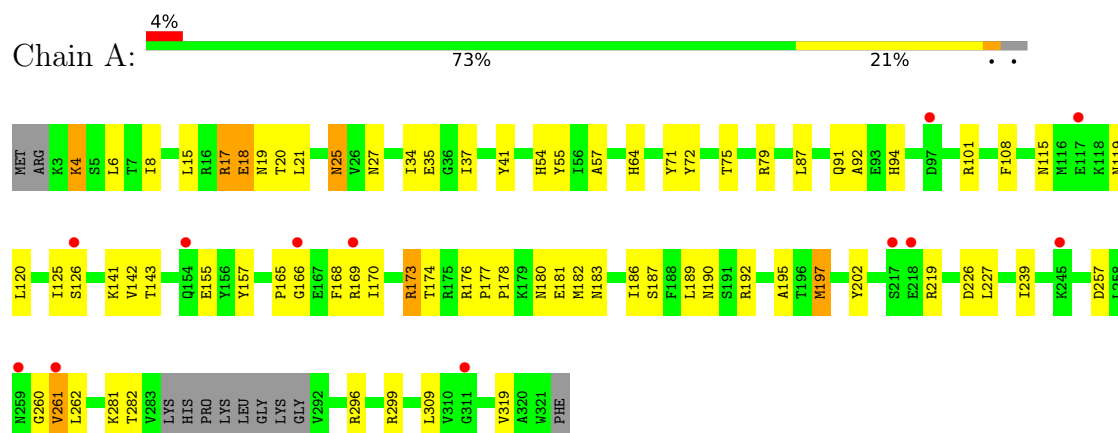
- Molecule 2 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	Q	84	Total	C	H	N	O	S	0	0	0
			1401	447	708	116	127	3			
2	R	84	Total	C	H	N	O	S	0	0	0
			1413	447	720	116	127	3			
2	S	84	Total	C	H	N	O	S	0	0	0
			1413	447	720	116	127	3			
2	T	84	Total	C	H	N	O	S	0	0	0
			1413	447	720	116	127	3			
2	U	84	Total	C	H	N	O	S	0	0	0
			1412	447	719	116	127	3			
2	V	84	Total	C	H	N	O	S	0	0	0
			1411	447	718	116	127	3			
2	W	84	Total	C	H	N	O	S	0	0	0
			1413	447	720	116	127	3			
2	X	84	Total	C	H	N	O	S	0	0	0
			1411	447	718	116	127	3			

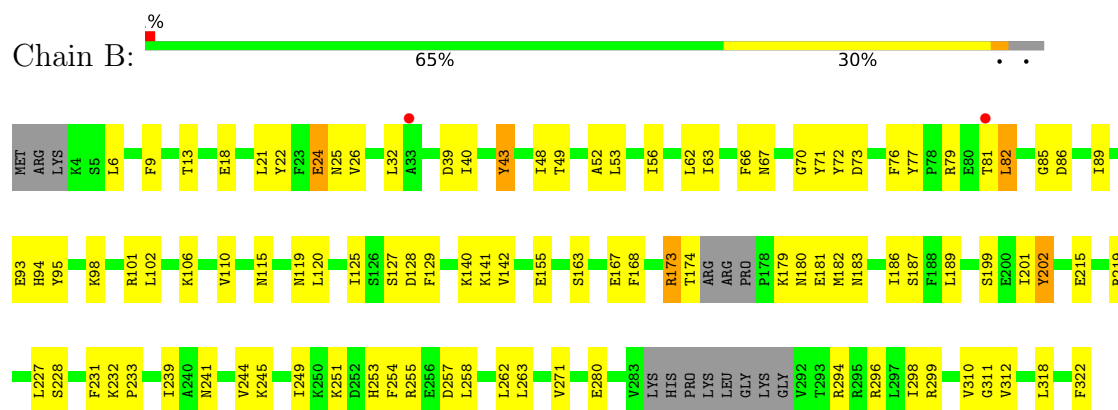
3 Residue-property plots

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 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.

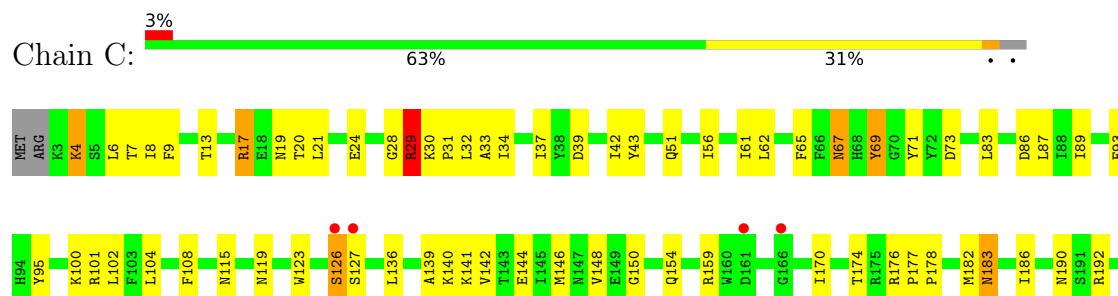
• Molecule 1: CRISPR-associated endonuclease Cas1

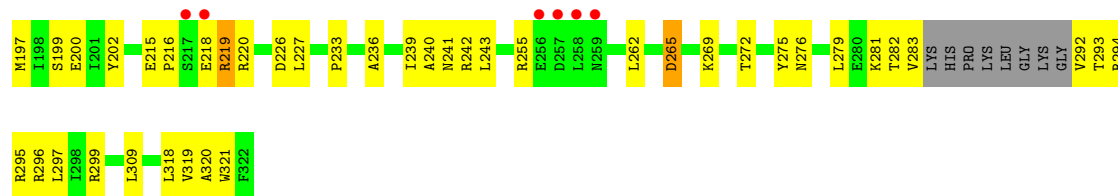


• Molecule 1: CRISPR-associated endonuclease Cas1



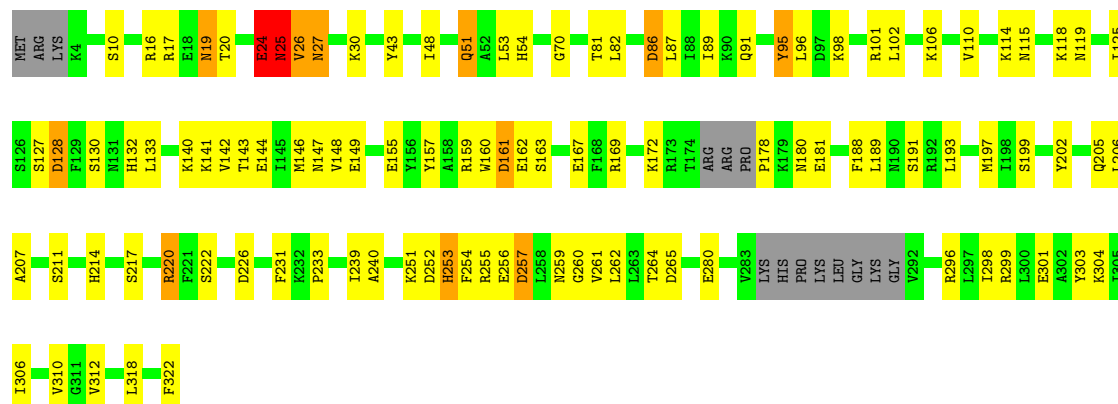
• Molecule 1: CRISPR-associated endonuclease Cas1





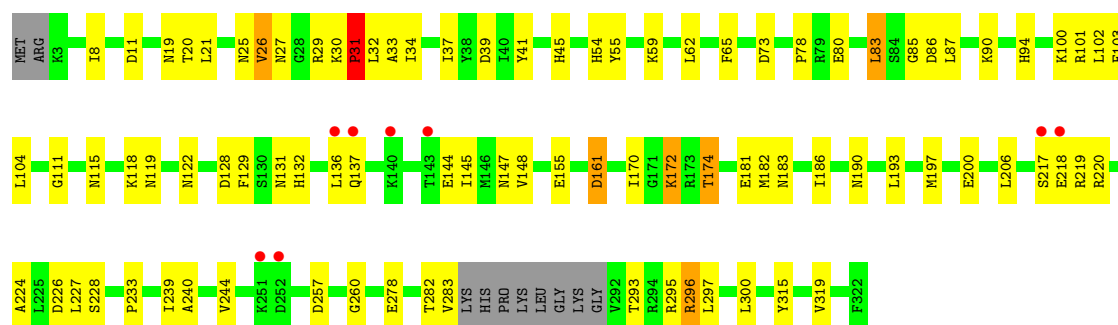
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain D: 63% 29%



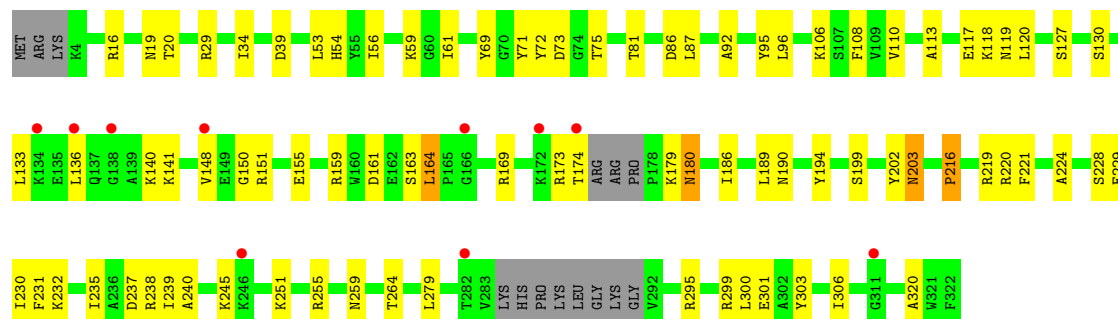
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain E: 2% 69% 26%

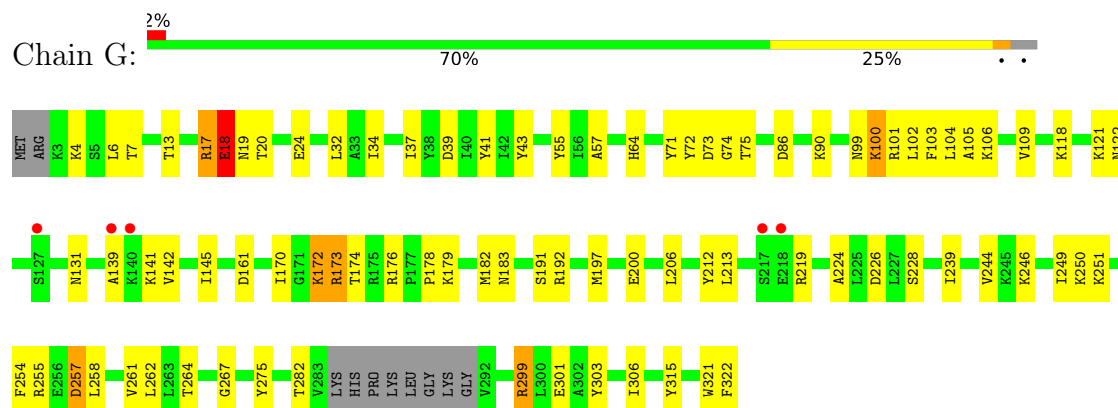


• Molecule 1: CRISPR-associated endonuclease Cas1

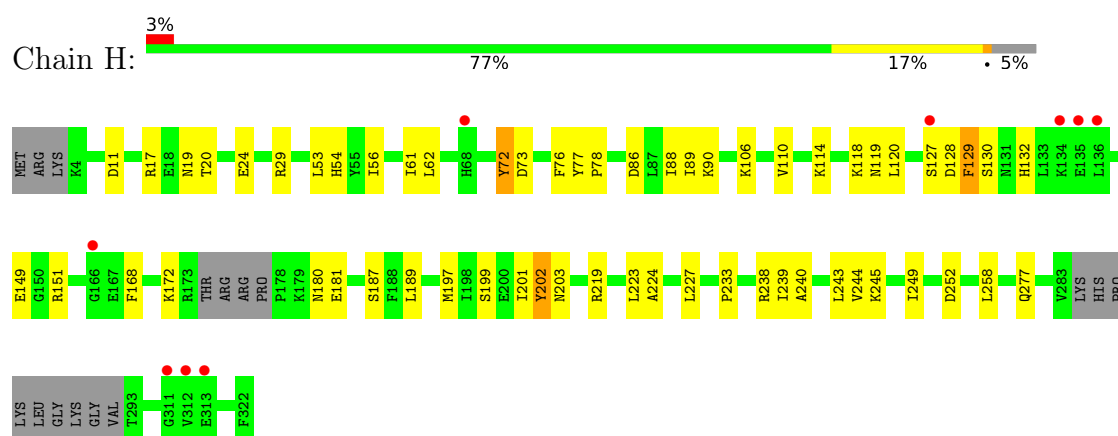
Chain F: 3% 70% 25%



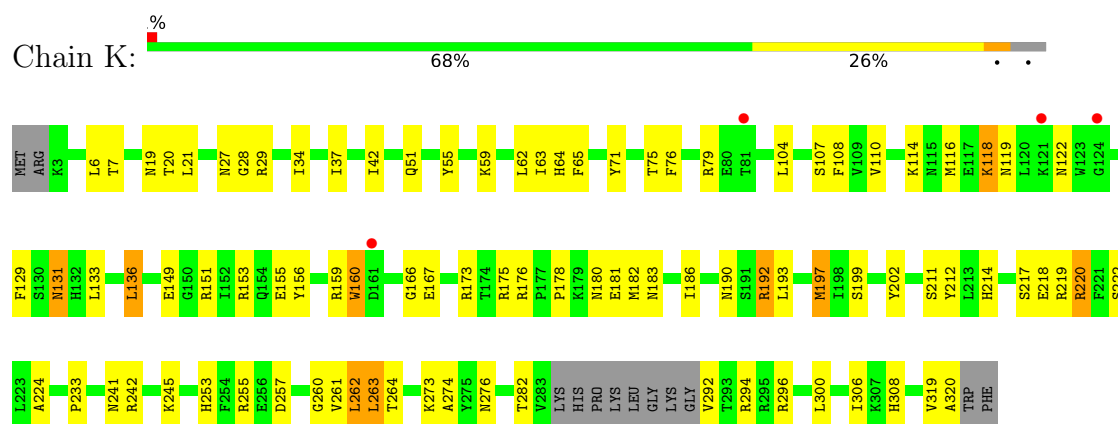
• Molecule 1: CRISPR-associated endonuclease Cas1



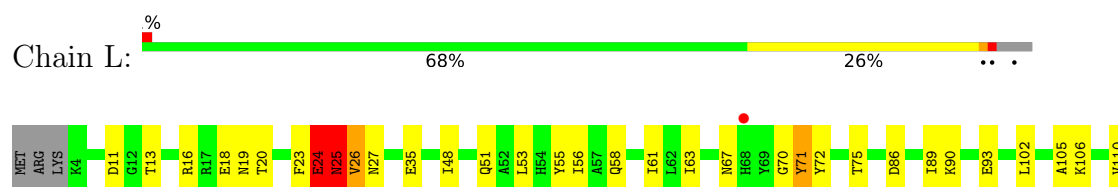
• Molecule 1: CRISPR-associated endonuclease Cas1

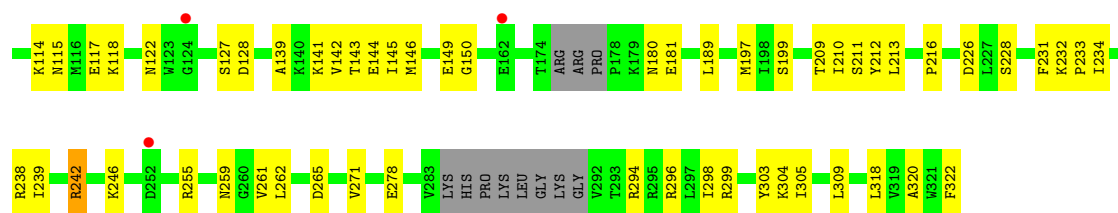


• Molecule 1: CRISPR-associated endonuclease Cas1

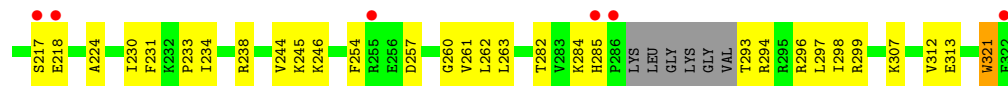
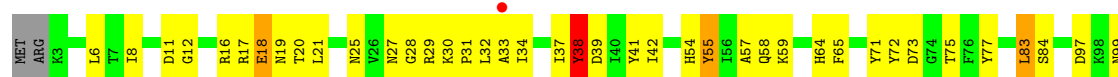


• Molecule 1: CRISPR-associated endonuclease Cas1

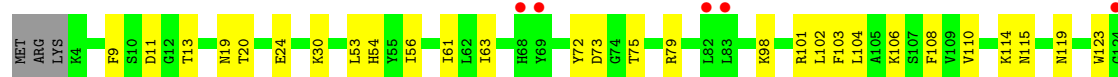
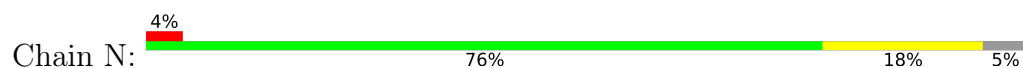




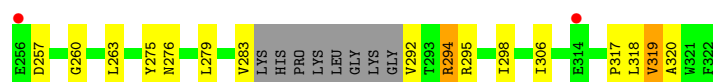
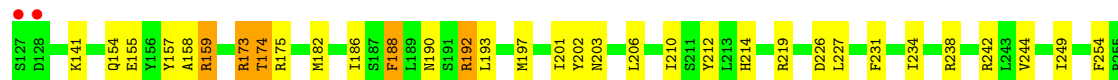
• Molecule 1: CRISPR-associated endonuclease Cas1



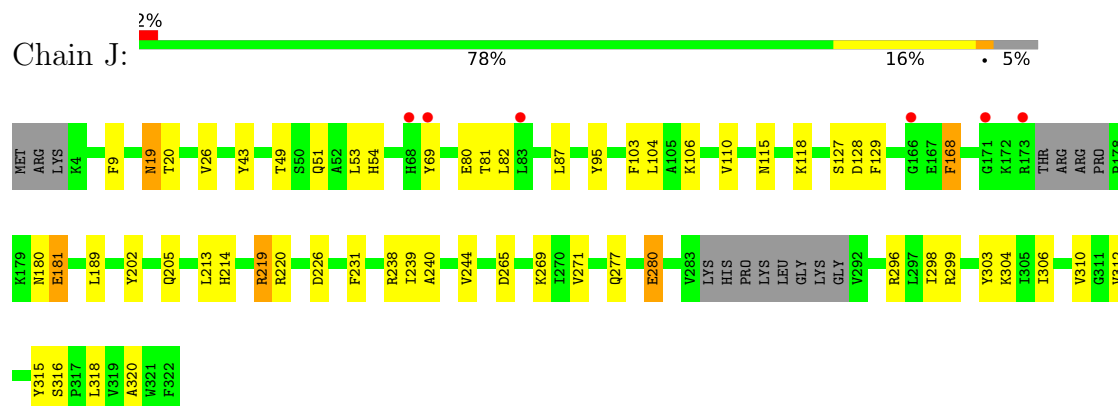
• Molecule 1: CRISPR-associated endonuclease Cas1



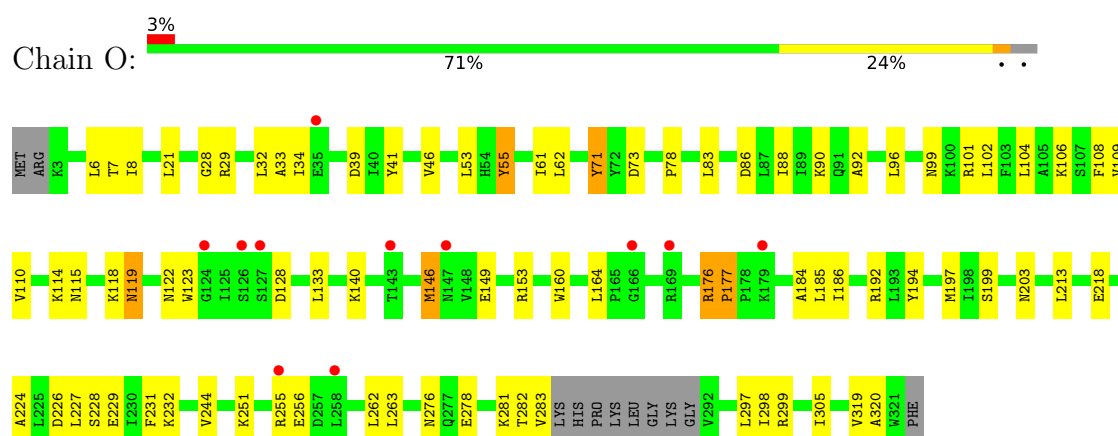
• Molecule 1: CRISPR-associated endonuclease Cas1



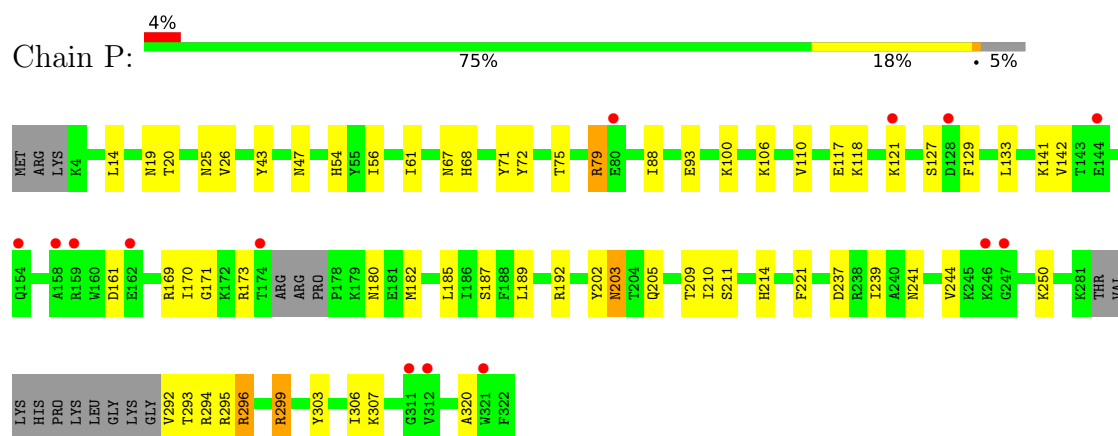
- Molecule 1: CRISPR-associated endonuclease Cas1



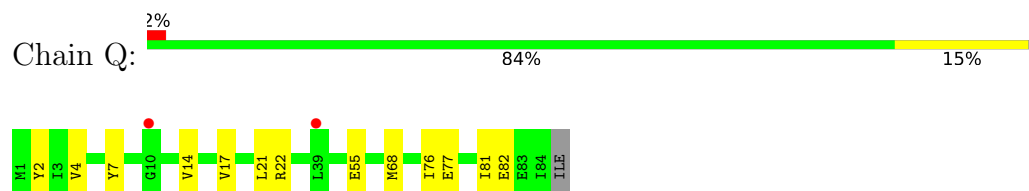
- Molecule 1: CRISPR-associated endonuclease Cas1



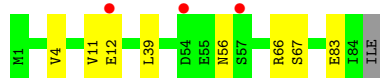
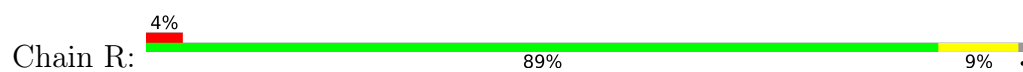
- Molecule 1: CRISPR-associated endonuclease Cas1



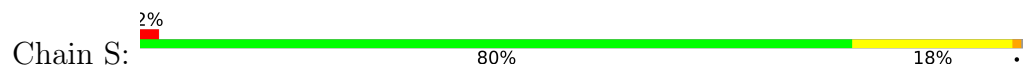
- Molecule 2: CRISPR-associated endoribonuclease Cas2



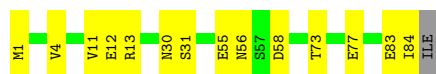
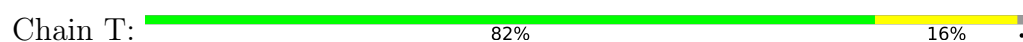
- Molecule 2: CRISPR-associated endoribonuclease Cas2



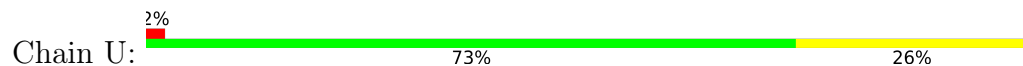
- Molecule 2: CRISPR-associated endoribonuclease Cas2



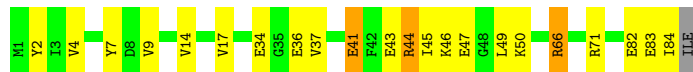
- Molecule 2: CRISPR-associated endoribonuclease Cas2



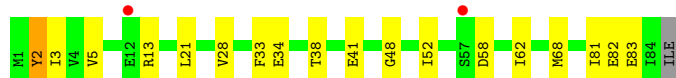
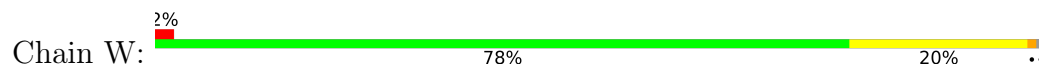
- Molecule 2: CRISPR-associated endoribonuclease Cas2



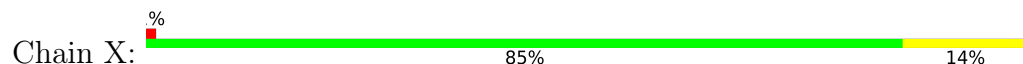
- Molecule 2: CRISPR-associated endoribonuclease Cas2



- Molecule 2: CRISPR-associated endoribonuclease Cas2



- Molecule 2: CRISPR-associated endoribonuclease Cas2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.76Å 180.47Å 338.85Å 90.00° 94.43° 90.00°	Depositor
Resolution (Å)	36.53 – 3.90 37.58 – 3.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (36.53-3.90) 93.7 (37.58-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 3.87Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.281 , 0.328 0.281 , (Not available)	Depositor DCC
R_{free} test set	971 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	90949	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.8394e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.27	0/2612	0.54	1/3517 (0.0%)
1	B	0.26	0/2584	0.51	0/3478
1	C	0.28	0/2624	0.50	0/3533
1	D	0.27	0/2584	0.52	1/3478 (0.0%)
1	E	0.28	0/2624	0.52	2/3533 (0.1%)
1	F	0.26	0/2584	0.48	0/3478
1	G	0.27	0/2624	0.50	0/3533
1	H	0.27	0/2570	0.47	0/3458
1	I	0.30	0/2624	0.54	0/3533
1	J	0.25	0/2577	0.45	0/3468
1	K	0.28	0/2596	0.53	0/3494
1	L	0.26	0/2584	0.51	0/3478
1	M	0.36	1/2645 (0.0%)	0.53	0/3561
1	N	0.25	0/2560	0.46	0/3443
1	O	0.27	0/2612	0.49	0/3517
1	P	0.25	0/2570	0.45	0/3458
2	Q	0.26	0/704	0.45	0/947
2	R	0.26	0/704	0.44	0/947
2	S	0.27	0/704	0.46	0/947
2	T	0.29	0/704	0.50	1/947 (0.1%)
2	U	0.26	0/704	0.48	0/947
2	V	0.27	0/704	0.48	0/947
2	W	0.26	0/704	0.46	0/947
2	X	0.26	0/704	0.45	0/947
All	All	0.27	1/47206 (0.0%)	0.50	5/63536 (0.0%)

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	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	3
1	E	0	3
1	F	0	1
1	G	0	4
1	I	0	2
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	2
1	O	0	1
All	All	0	21

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	38	TYR	CD2-CE2	-7.43	1.28	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	261	VAL	CG1-CB-CG2	8.11	123.88	110.90
1	A	261	VAL	CG1-CB-CG2	7.42	122.78	110.90
2	T	4	VAL	CG1-CB-CG2	5.15	119.14	110.90
1	E	26	VAL	CA-CB-CG2	5.14	118.61	110.90
1	E	31	PRO	N-CA-C	5.02	125.14	112.10

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	ARG	Peptide
1	C	17	ARG	Peptide
1	D	149	GLU	Peptide
1	D	24	GLU	Peptide
1	D	25	ASN	Peptide

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	2559	2443	2609	69	0
1	B	2532	2409	2572	73	1
1	C	2570	2450	2618	101	0
1	D	2532	2405	2572	72	1
1	E	2570	2433	2618	83	0
1	F	2532	2418	2572	63	1
1	G	2570	2446	2618	63	0
1	H	2518	2408	2556	42	1
1	I	2570	2467	2618	78	0
1	J	2525	2399	2565	38	1
1	K	2545	2467	2599	71	0
1	L	2532	2426	2572	67	1
1	M	2589	2481	2636	94	0
1	N	2509	2396	2550	42	1
1	O	2559	2465	2609	80	0
1	P	2518	2419	2556	47	1
2	Q	693	708	721	9	0
2	R	693	720	721	7	0
2	S	693	720	721	11	0
2	T	693	720	721	9	0
2	U	693	719	721	15	0
2	V	693	718	721	17	0
2	W	693	720	721	14	0
2	X	693	718	721	9	0
All	All	46274	44675	47208	1085	4

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 12.

The worst 5 of 1085 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:4:LYS:NZ	2:Q:77:GLU:OE2	1.74	1.21
1:K:133:LEU:O	1:K:136:LEU:CD2	1.99	1.10
1:L:278:GLU:OE2	1:L:294:ARG:NH1	1.85	1.09
1:K:133:LEU:O	1:K:136:LEU:HD22	1.55	1.06
1:M:38:TYR:OH	1:M:299:ARG:NH1	1.88	1.06

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:252:ASP:O	1:J:219:ARG:NH1[1_455]	1.86	0.34
1:B:187:SER:OG	1:F:259:ASN:ND2[1_655]	2.06	0.14
1:D:259:ASN:HD21	1:H:187:SER:O[1_455]	1.57	0.03
1:L:259:ASN:HD21	1:P:187:SER:O[1_455]	1.58	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
1	A	307/322 (95%)	285 (93%)	21 (7%)	1 (0%)	41	75
1	B	302/322 (94%)	275 (91%)	25 (8%)	2 (1%)	22	60
1	C	308/322 (96%)	278 (90%)	26 (8%)	4 (1%)	12	48
1	D	302/322 (94%)	274 (91%)	21 (7%)	7 (2%)	6	38
1	E	308/322 (96%)	288 (94%)	19 (6%)	1 (0%)	41	75
1	F	302/322 (94%)	273 (90%)	28 (9%)	1 (0%)	41	75
1	G	308/322 (96%)	279 (91%)	27 (9%)	2 (1%)	25	63
1	H	300/322 (93%)	287 (96%)	12 (4%)	1 (0%)	41	75
1	I	308/322 (96%)	282 (92%)	21 (7%)	5 (2%)	9	44
1	J	301/322 (94%)	279 (93%)	22 (7%)	0	100	100
1	K	306/322 (95%)	279 (91%)	26 (8%)	1 (0%)	41	75
1	L	302/322 (94%)	267 (88%)	32 (11%)	3 (1%)	15	52
1	M	310/322 (96%)	275 (89%)	34 (11%)	1 (0%)	41	75
1	N	297/322 (92%)	273 (92%)	24 (8%)	0	100	100
1	O	307/322 (95%)	282 (92%)	24 (8%)	1 (0%)	41	75
1	P	300/322 (93%)	283 (94%)	16 (5%)	1 (0%)	41	75
2	Q	82/85 (96%)	76 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	R	82/85 (96%)	74 (90%)	8 (10%)	0	100	100
2	S	82/85 (96%)	75 (92%)	7 (8%)	0	100	100
2	T	82/85 (96%)	77 (94%)	5 (6%)	0	100	100
2	U	82/85 (96%)	77 (94%)	5 (6%)	0	100	100
2	V	82/85 (96%)	76 (93%)	6 (7%)	0	100	100
2	W	82/85 (96%)	71 (87%)	11 (13%)	0	100	100
2	X	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
All	All	5524/5832 (95%)	5066 (92%)	427 (8%)	31 (1%)	25	63

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	B	128	ASP
1	D	25	ASN
1	D	26	VAL
1	D	257	ASP

5.3.2 Protein sidechains ⓘ

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	
1	A	275/284 (97%)	267 (97%)	8 (3%)	42	65
1	B	272/284 (96%)	259 (95%)	13 (5%)	25	54
1	C	276/284 (97%)	257 (93%)	19 (7%)	15	45
1	D	272/284 (96%)	257 (94%)	15 (6%)	21	51
1	E	276/284 (97%)	268 (97%)	8 (3%)	42	65
1	F	272/284 (96%)	261 (96%)	11 (4%)	31	58
1	G	276/284 (97%)	264 (96%)	12 (4%)	29	57
1	H	270/284 (95%)	262 (97%)	8 (3%)	41	64
1	I	276/284 (97%)	265 (96%)	11 (4%)	31	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	271/284 (95%)	261 (96%)	10 (4%)	34	60
1	K	274/284 (96%)	259 (94%)	15 (6%)	21	51
1	L	272/284 (96%)	265 (97%)	7 (3%)	46	68
1	M	278/284 (98%)	266 (96%)	12 (4%)	29	57
1	N	269/284 (95%)	264 (98%)	5 (2%)	57	75
1	O	275/284 (97%)	269 (98%)	6 (2%)	52	71
1	P	270/284 (95%)	260 (96%)	10 (4%)	34	60
2	Q	79/80 (99%)	78 (99%)	1 (1%)	69	82
2	R	79/80 (99%)	79 (100%)	0	100	100
2	S	79/80 (99%)	76 (96%)	3 (4%)	33	59
2	T	79/80 (99%)	78 (99%)	1 (1%)	69	82
2	U	79/80 (99%)	76 (96%)	3 (4%)	33	59
2	V	79/80 (99%)	76 (96%)	3 (4%)	33	59
2	W	79/80 (99%)	78 (99%)	1 (1%)	69	82
2	X	79/80 (99%)	78 (99%)	1 (1%)	69	82
All	All	5006/5184 (97%)	4823 (96%)	183 (4%)	34	60

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	182	MET
1	N	30	LYS
1	K	220	ARG
1	M	30	LYS
1	I	173	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	308	HIS
1	P	308	HIS
1	M	115	ASN
1	J	308	HIS
1	L	308	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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, 95th 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	311/322 (96%)	0.16	12 (3%) 39 30	15, 49, 99, 125	0
1	B	308/322 (95%)	-0.09	2 (0%) 89 84	16, 43, 75, 116	0
1	C	312/322 (96%)	0.08	10 (3%) 47 37	10, 45, 94, 114	0
1	D	308/322 (95%)	-0.17	0 100 100	15, 38, 73, 105	0
1	E	312/322 (96%)	0.06	8 (2%) 56 45	11, 47, 87, 126	0
1	F	308/322 (95%)	0.12	10 (3%) 47 37	16, 60, 95, 109	0
1	G	312/322 (96%)	0.01	5 (1%) 72 62	8, 41, 88, 122	0
1	H	306/322 (95%)	0.07	9 (2%) 51 40	13, 54, 93, 106	0
1	I	312/322 (96%)	0.06	5 (1%) 72 62	12, 47, 81, 100	0
1	J	307/322 (95%)	0.11	6 (1%) 65 55	21, 58, 87, 107	0
1	K	310/322 (96%)	0.01	4 (1%) 77 68	11, 41, 79, 112	0
1	L	308/322 (95%)	0.11	4 (1%) 77 68	14, 52, 85, 103	0
1	M	314/322 (97%)	0.10	12 (3%) 40 31	13, 53, 91, 132	0
1	N	305/322 (94%)	0.35	12 (3%) 39 30	30, 70, 102, 117	0
1	O	311/322 (96%)	0.07	11 (3%) 44 34	9, 46, 89, 116	0
1	P	306/322 (95%)	0.26	14 (4%) 32 26	22, 67, 96, 120	0
2	Q	84/85 (98%)	0.15	2 (2%) 59 48	17, 49, 83, 88	0
2	R	84/85 (98%)	0.12	3 (3%) 42 33	12, 44, 71, 103	0
2	S	84/85 (98%)	0.06	2 (2%) 59 48	11, 44, 77, 102	0
2	T	84/85 (98%)	0.03	0 100 100	9, 40, 68, 94	0
2	U	84/85 (98%)	0.06	2 (2%) 59 48	15, 45, 92, 103	0
2	V	84/85 (98%)	-0.04	0 100 100	14, 47, 71, 81	0
2	W	84/85 (98%)	-0.03	2 (2%) 59 48	15, 40, 78, 102	0
2	X	84/85 (98%)	-0.01	1 (1%) 79 70	11, 42, 67, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
All	All	5622/5832 (96%)	0.08	136 (2%)	59 48	8, 50, 91, 132	0

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	258	LEU	4.5
1	P	311	GLY	4.5
1	N	68	HIS	4.0
1	H	68	HIS	3.8
1	O	143	THR	3.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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.