



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 26, 2022 – 09:13 pm BST

PDB ID : 2Y9H  
Title : Structure A of CRISPR endoribonuclease Cse3 bound to 19 nt RNA  
Authors : Sashital, D.G.; Jinek, M.; Doudna, J.A.  
Deposited on : 2011-02-14  
Resolution : 2.50 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](mailto: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 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:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

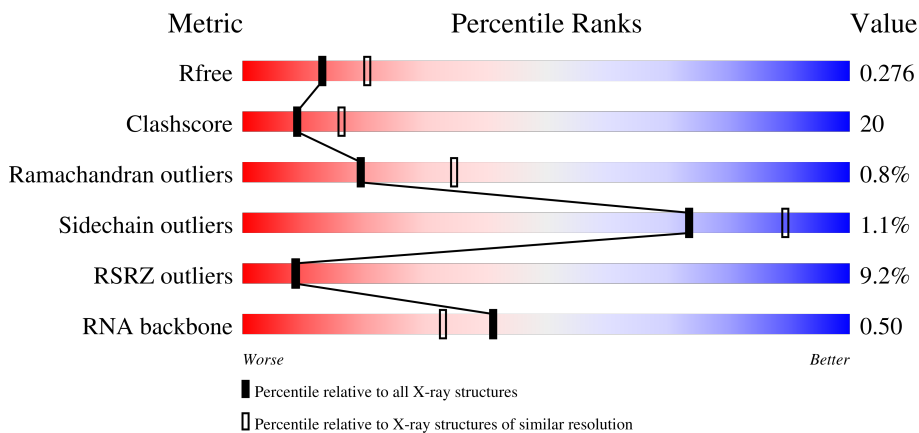
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	215	 4% 61% 38% 7%
1	C	215	 3% 64% 33% 2% 2%
1	E	215	 4% 54% 44% 2% 2%
1	G	215	 2% 66% 26% 2% 7%

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	215	
1	K	215	
1	M	215	
1	O	215	
2	B	19	
2	D	19	
2	F	19	
2	H	19	
2	J	19	
2	L	19	
2	N	19	
2	P	19	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15663 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 protein called CSE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	213	Total 1685	C 1074	N 319	O 290	S 2	0	0	0
1	C	211	Total 1676	C 1069	N 317	O 288	S 2	0	0	0
1	E	211	Total 1668	C 1064	N 316	O 286	S 2	0	0	0
1	G	199	Total 1587	C 1017	N 300	O 268	S 2	0	0	0
1	I	195	Total 1545	C 992	N 289	O 262	S 2	0	0	0
1	K	191	Total 1519	C 975	N 282	O 260	S 2	0	0	0
1	M	193	Total 1528	C 982	N 284	O 260	S 2	0	0	0
1	O	177	Total 908	C 554	N 177	O 177		0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q53WG9
A	-2	THR	-	expression tag	UNP Q53WG9
A	-1	GLY	-	expression tag	UNP Q53WG9
A	0	ALA	-	expression tag	UNP Q53WG9
C	-3	GLY	-	expression tag	UNP Q53WG9
C	-2	THR	-	expression tag	UNP Q53WG9
C	-1	GLY	-	expression tag	UNP Q53WG9
C	0	ALA	-	expression tag	UNP Q53WG9
E	-3	GLY	-	expression tag	UNP Q53WG9
E	-2	THR	-	expression tag	UNP Q53WG9
E	-1	GLY	-	expression tag	UNP Q53WG9
E	0	ALA	-	expression tag	UNP Q53WG9
G	-3	GLY	-	expression tag	UNP Q53WG9

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	THR	-	expression tag	UNP Q53WG9
G	-1	GLY	-	expression tag	UNP Q53WG9
G	0	ALA	-	expression tag	UNP Q53WG9
I	-3	GLY	-	expression tag	UNP Q53WG9
I	-2	THR	-	expression tag	UNP Q53WG9
I	-1	GLY	-	expression tag	UNP Q53WG9
I	0	ALA	-	expression tag	UNP Q53WG9
K	-3	GLY	-	expression tag	UNP Q53WG9
K	-2	THR	-	expression tag	UNP Q53WG9
K	-1	GLY	-	expression tag	UNP Q53WG9
K	0	ALA	-	expression tag	UNP Q53WG9
M	-3	GLY	-	expression tag	UNP Q53WG9
M	-2	THR	-	expression tag	UNP Q53WG9
M	-1	GLY	-	expression tag	UNP Q53WG9
M	0	ALA	-	expression tag	UNP Q53WG9
O	-3	GLY	-	expression tag	UNP Q53WG9
O	-2	THR	-	expression tag	UNP Q53WG9
O	-1	GLY	-	expression tag	UNP Q53WG9
O	0	ALA	-	expression tag	UNP Q53WG9

- Molecule 2 is a RNA chain called 5'-R(\*UP\*CP\*CP\*CP\*CP\*AP\*CP\*GP\*CP\*GP\*UP\*GP\*UP\*GP \*GP\*GP\*DGP\*AP\*UP)-3'.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
			Total	C	N	O				P
2	B	19	Total 385	C 171	N 69	O 127	P 18	0	0	0
2	D	19	Total 385	C 171	N 69	O 127	P 18	0	0	0
2	F	19	Total 385	C 171	N 69	O 127	P 18	0	0	0
2	H	19	Total 385	C 171	N 69	O 127	P 18	0	0	0
2	J	19	Total 385	C 171	N 69	O 127	P 18	0	0	0
2	L	19	Total 385	C 171	N 69	O 127	P 18	0	0	0
2	N	18	Total 381	C 171	N 69	O 124	P 17	0	0	0
2	P	18	Total 381	C 171	N 69	O 124	P 17	0	0	0

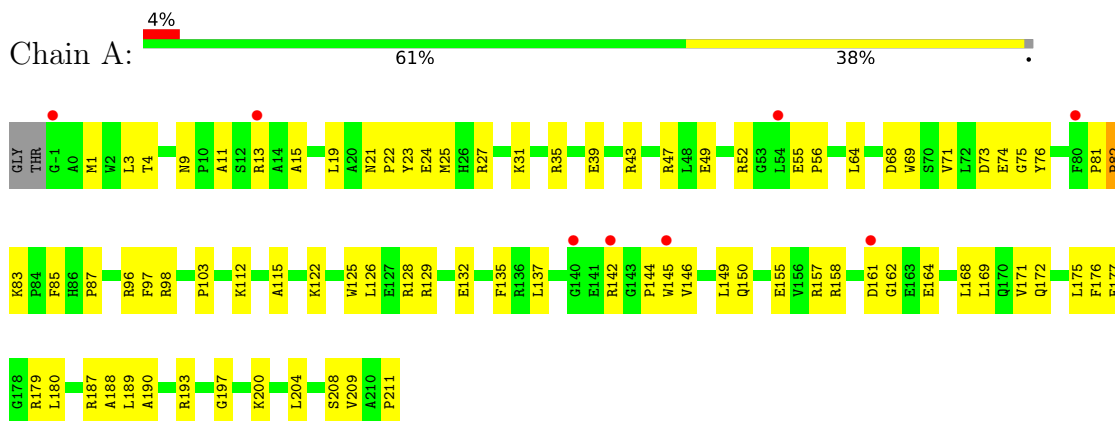
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	13	Total 13	O 13	0	0
3	C	30	Total 30	O 30	0	0
3	D	19	Total 19	O 19	0	0
3	E	51	Total 51	O 51	0	0
3	F	25	Total 25	O 25	0	0
3	G	30	Total 30	O 30	0	0
3	H	13	Total 13	O 13	0	0
3	I	57	Total 57	O 57	0	0
3	J	24	Total 24	O 24	0	0
3	K	56	Total 56	O 56	0	0
3	L	20	Total 20	O 20	0	0
3	M	44	Total 44	O 44	0	0
3	N	23	Total 23	O 23	0	0
3	O	22	Total 22	O 22	0	0
3	P	13	Total 13	O 13	0	0

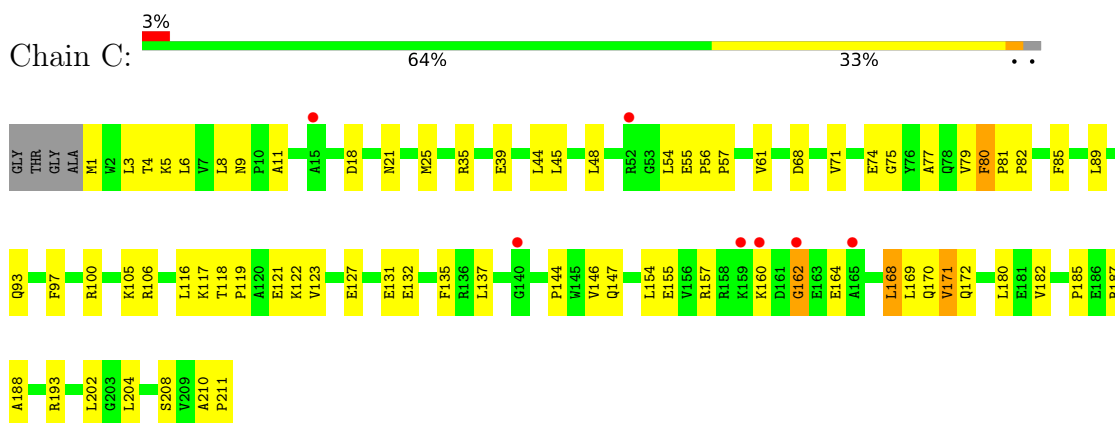
### 3 Residue-property plots [i](#)

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: CSE3



- Molecule 1: CSE3

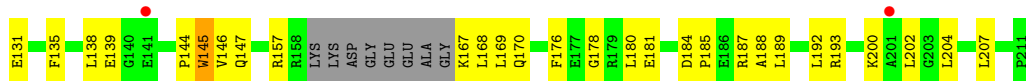
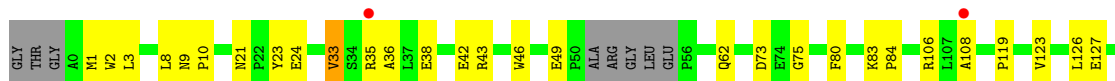


- Molecule 1: CSE3

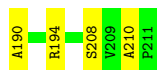
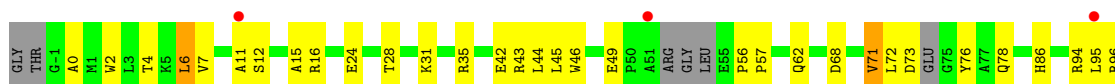




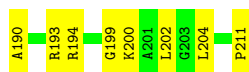
- Molecule 1: CSE3



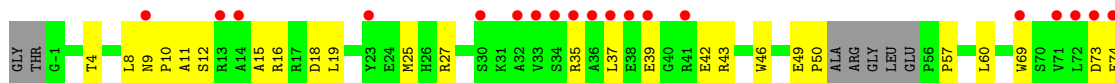
- Molecule 1: CSE3



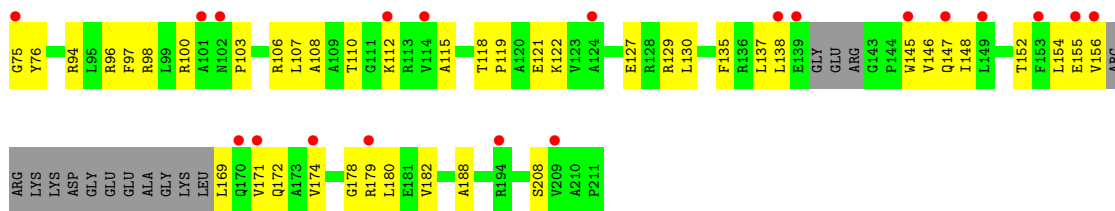
- Molecule 1: CSE3



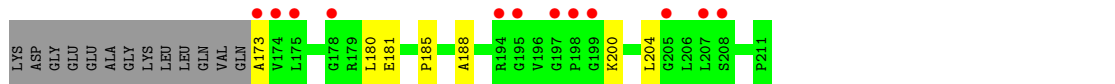
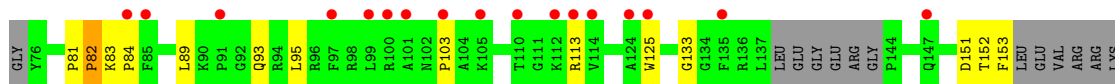
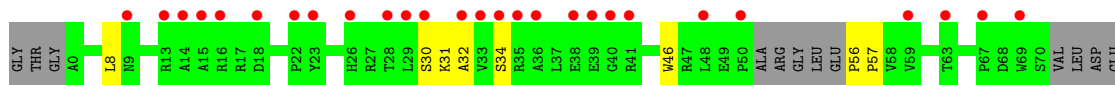
- Molecule 1: CSE3



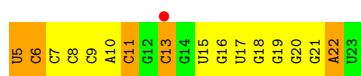
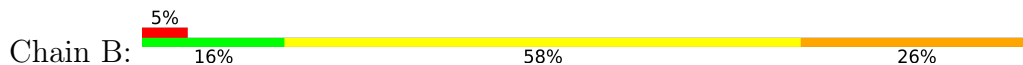




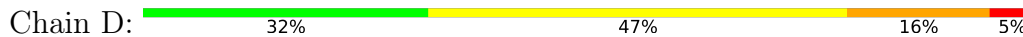
● Molecule 1: CSE3



● Molecule 2: 5'-R(\*UP\*CP\*CP\*CP\*CP\*AP\*CP\*GP\*CP\*GP\*UP\*GP\*UP\*GP \*GP\*GP\*DGP\*AP\*UP)-3'



● Molecule 2: 5'-R(\*UP\*CP\*CP\*CP\*CP\*AP\*CP\*GP\*CP\*GP\*UP\*GP\*UP\*GP \*GP\*GP\*DGP\*AP\*UP)-3'

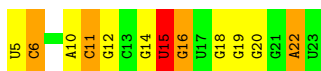


● Molecule 2: 5'-R(\*UP\*CP\*CP\*CP\*CP\*AP\*CP\*GP\*CP\*GP\*UP\*GP\*UP\*GP \*GP\*GP\*DGP\*AP\*UP)-3'

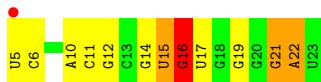


● Molecule 2: 5'-R(\*UP\*CP\*CP\*CP\*CP\*AP\*CP\*GP\*CP\*GP\*UP\*GP\*UP\*GP \*GP\*GP\*DGP\*AP\*UP)-3'

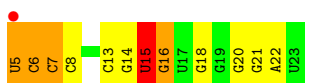




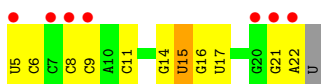
● Molecule 2: 5'-R(\*UP\*CP\*CP\*CP\*CP\*AP\*CP\*GP\*CP\*GP\*UP\*GP\*UP\*GP \*GP\*GP\*DGP\*AP\*UP)-3'



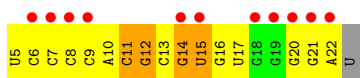
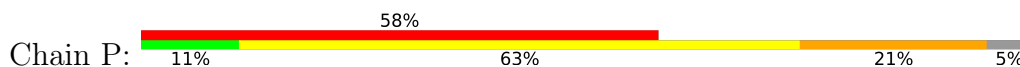
● Molecule 2: 5'-R(\*UP\*CP\*CP\*CP\*CP\*AP\*CP\*GP\*CP\*GP\*UP\*GP\*UP\*GP \*GP\*GP\*DGP\*AP\*UP)-3'



● Molecule 2: 5'-R(\*UP\*CP\*CP\*CP\*CP\*AP\*CP\*GP\*CP\*GP\*UP\*GP\*UP\*GP \*GP\*GP\*DGP\*AP\*UP)-3'



● Molecule 2: 5'-R(\*UP\*CP\*CP\*CP\*CP\*AP\*CP\*GP\*CP\*GP\*UP\*GP\*UP\*GP \*GP\*GP\*DGP\*AP\*UP)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.86Å 149.81Å 87.26Å 90.00° 94.60° 90.00°	Depositor
Resolution (Å)	58.70 – 2.50 58.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.70-2.50) 99.9 (58.70-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.40Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.231 , 0.289 0.219 , 0.276	Depositor DCC
$R_{free}$ test set	1994 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtrriage
Anisotropy	0.140	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15663	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.85 % 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 2.5178e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 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	0.46	0/1721	0.62	0/2329
1	C	0.47	0/1712	0.63	0/2317
1	E	0.52	0/1703	0.65	0/2304
1	G	0.45	0/1621	0.63	0/2194
1	I	0.50	0/1577	0.67	0/2135
1	K	0.49	0/1552	0.65	0/2103
1	M	0.41	0/1561	0.59	0/2115
1	O	0.32	0/920	0.53	0/1285
2	B	0.99	1/429 (0.2%)	1.10	2/668 (0.3%)
2	D	1.18	6/429 (1.4%)	1.12	0/668
2	F	1.23	7/429 (1.6%)	1.38	9/668 (1.3%)
2	H	1.08	4/429 (0.9%)	1.14	3/668 (0.4%)
2	J	0.72	0/429	1.49	6/668 (0.9%)
2	L	0.62	0/429	1.26	5/668 (0.7%)
2	N	0.50	0/425	0.98	0/661
2	P	0.37	0/425	0.90	0/661
All	All	0.58	18/15791 (0.1%)	0.80	25/22112 (0.1%)

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	22	A	N7-C5	-9.25	1.33	1.39
2	H	22	A	N7-C5	-8.97	1.33	1.39
2	D	22	A	N3-C4	-8.51	1.29	1.34
2	D	22	A	N7-C5	-7.35	1.34	1.39
2	D	22	A	C6-N1	-7.20	1.30	1.35

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	16	G	C5-N7-C8	-9.87	99.37	104.30
2	J	21	DG	O4'-C1'-N9	9.60	114.72	108.00
2	J	16	G	C4-C5-N7	9.46	114.58	110.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	22	A	O4'-C1'-C2'	-7.98	97.82	105.80
2	H	15	U	C2-N1-C1'	7.93	127.22	117.70

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	1685	0	1762	98	0
1	C	1676	0	1754	71	1
1	E	1668	0	1744	95	0
1	G	1587	0	1667	48	0
1	I	1545	0	1615	45	0
1	K	1519	0	1582	61	0
1	M	1528	0	1597	65	0
1	O	908	0	513	15	0
2	B	385	0	196	27	0
2	D	385	0	196	23	0
2	F	385	0	196	21	0
2	H	385	0	196	13	0
2	J	385	0	196	18	0
2	L	385	0	196	15	0
2	N	381	0	197	18	0
2	P	381	0	197	19	0
3	A	35	0	0	3	0
3	B	13	0	0	3	0
3	C	30	0	0	1	1
3	D	19	0	0	0	0
3	E	51	0	0	7	2
3	F	25	0	0	3	0
3	G	30	0	0	3	0
3	H	13	0	0	2	0
3	I	57	0	0	5	0
3	J	24	0	0	2	0
3	K	56	0	0	3	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	20	0	0	1	0
3	M	44	0	0	2	0
3	N	23	0	0	5	0
3	O	22	0	0	2	0
3	P	13	0	0	0	0
All	All	15663	0	13804	584	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 20.

The worst 5 of 584 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:K:74:GLU:HA	1:K:76:TYR:H	1.08	1.17
1:K:74:GLU:HG3	1:K:75:GLY:HA2	1.25	1.14
2:J:21:DG:C2'	2:J:22:A:H5'	1.92	0.99
1:A:83:LYS:HE2	2:F:9:C:OP1	1.63	0.97
1:A:145:TRP:CD1	1:A:179:ARG:HB2	2.00	0.95

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)
3:C:2021:HOH:O	3:E:2020:HOH:O[2_445]	2.01	0.19
1:C:155:GLU:OE2	3:E:2026:HOH:O[2_445]	2.16	0.04

## 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
1	A	211/215 (98%)	198 (94%)	12 (6%)	1 (0%)	29 48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	209/215 (97%)	194 (93%)	14 (7%)	1 (0%)	29	48
1	E	207/215 (96%)	196 (95%)	10 (5%)	1 (0%)	29	48
1	G	193/215 (90%)	185 (96%)	5 (3%)	3 (2%)	9	17
1	I	185/215 (86%)	175 (95%)	10 (5%)	0	100	100
1	K	183/215 (85%)	174 (95%)	7 (4%)	2 (1%)	14	26
1	M	185/215 (86%)	174 (94%)	11 (6%)	0	100	100
1	O	167/215 (78%)	139 (83%)	24 (14%)	4 (2%)	6	9
All	All	1540/1720 (90%)	1435 (93%)	93 (6%)	12 (1%)	19	35

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	33	VAL
1	K	145	TRP
1	O	8	LEU
1	O	31	LYS
1	O	34	SER

### 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	
1	A	172/173 (99%)	172 (100%)	0	100	100
1	C	172/173 (99%)	167 (97%)	5 (3%)	42	69
1	E	170/173 (98%)	168 (99%)	2 (1%)	71	88
1	G	164/173 (95%)	162 (99%)	2 (1%)	71	88
1	I	159/173 (92%)	155 (98%)	4 (2%)	47	73
1	K	157/173 (91%)	157 (100%)	0	100	100
1	M	158/173 (91%)	158 (100%)	0	100	100
1	O	17/173 (10%)	17 (100%)	0	100	100
All	All	1169/1384 (84%)	1156 (99%)	13 (1%)	73	89

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	46	TRP
1	G	187	ARG
1	I	168	LEU
1	I	71	VAL
1	I	94	ARG

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	93	GLN
1	G	147	GLN
1	I	86	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	17/19 (89%)	5 (29%)	1 (5%)
2	D	16/19 (84%)	4 (25%)	1 (6%)
2	F	16/19 (84%)	6 (37%)	1 (6%)
2	H	16/19 (84%)	6 (37%)	1 (6%)
2	J	16/19 (84%)	3 (18%)	1 (6%)
2	L	17/19 (89%)	6 (35%)	2 (11%)
2	N	16/19 (84%)	3 (18%)	0
2	P	16/19 (84%)	6 (37%)	2 (12%)
All	All	130/152 (85%)	39 (30%)	9 (6%)

5 of 39 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	6	C
2	B	11	C
2	B	13	C
2	B	15	U
2	B	16	G

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	P	12	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	P	14	G
2	H	15	U
2	J	15	U
2	L	5	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 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	213/215 (99%)	0.41	8 (3%) 40 43	23, 41, 78, 118	0
1	C	211/215 (98%)	0.36	7 (3%) 46 50	21, 41, 82, 115	0
1	E	211/215 (98%)	0.36	8 (3%) 40 43	18, 41, 75, 112	0
1	G	199/215 (92%)	0.29	4 (2%) 65 68	21, 41, 64, 95	0
1	I	195/215 (90%)	0.26	9 (4%) 32 34	12, 32, 64, 98	0
1	K	191/215 (88%)	0.28	8 (4%) 36 39	15, 35, 63, 99	0
1	M	193/215 (89%)	1.11	39 (20%) 1 0	27, 47, 78, 109	0
1	O	177/215 (82%)	1.49	56 (31%) 0 0	63, 85, 116, 132	0
2	B	19/19 (100%)	0.18	1 (5%) 26 28	43, 57, 104, 110	0
2	D	19/19 (100%)	0.44	0 100 100	36, 52, 68, 69	0
2	F	19/19 (100%)	0.25	0 100 100	34, 42, 58, 74	0
2	H	19/19 (100%)	0.25	0 100 100	41, 55, 72, 84	0
2	J	19/19 (100%)	0.54	1 (5%) 26 28	25, 37, 104, 118	0
2	L	19/19 (100%)	0.35	1 (5%) 26 28	28, 46, 88, 148	0
2	N	18/19 (94%)	1.43	7 (38%) 0 0	41, 57, 87, 99	0
2	P	18/19 (94%)	2.45	11 (61%) 0 0	116, 128, 162, 176	0
All	All	1740/1872 (92%)	0.57	160 (9%) 9 9	12, 43, 95, 176	0

The worst 5 of 160 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	ARG	9.0
1	O	101	ALA	7.9
2	J	5	U	7.0
2	P	22	A	6.5
1	O	178	GLY	6.3

## 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.