



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2023 – 03:54 PM EDT

PDB ID : 2Q4G  
Title : Ensemble refinement of the protein crystal structure of human ribonuclease inhibitor complexed with ribonuclease I  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 1.95 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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

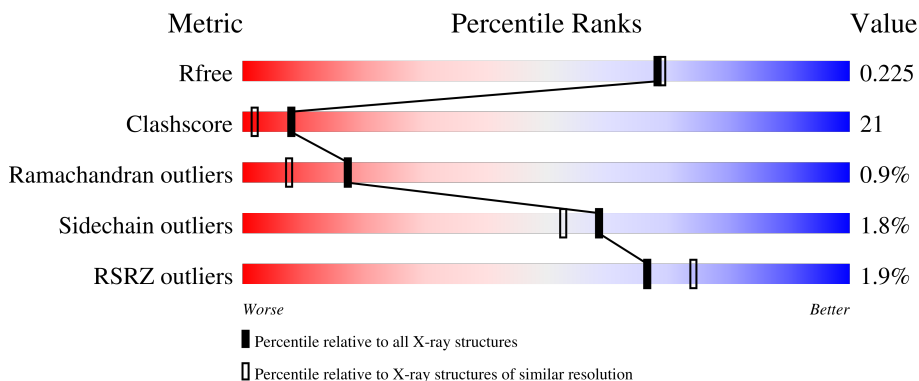
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	1-X	129	 7% 67% 29% ..
1	1-Z	129	 % 61% 36% .
1	2-X	129	 7% 78% 20% .
1	2-Z	129	 % 67% 31% .
1	3-X	129	 7% 74% 22% ...

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Mol	Chain	Length	Quality of chain	
1	3-Z	129		..
1	4-X	129		..
1	4-Z	129		..
1	5-X	129		..
1	5-Z	129		..
1	6-X	129		..
1	6-Z	129		.
1	7-X	129		..
1	7-Z	129		..
1	8-X	129		..
1	8-Z	129		..
2	1-W	461		.
2	1-Y	461		.
2	2-W	461		.
2	2-Y	461		.
2	3-W	461		.
2	3-Y	461		.
2	4-W	461		.
2	4-Y	461		.
2	5-W	461		.
2	5-Y	461		.
2	6-W	461		.
2	6-Y	461		.
2	7-W	461		.
2	7-Y	461		.

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Mol	Chain	Length	Quality of chain
2	8-W	461	<p>%</p> <p>70% 29%</p>
2	8-Y	461	<p>2%</p> <p>66% 33%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CIT	1-X	900	-	X	-	-
3	CIT	2-X	900	-	X	-	-
3	CIT	3-X	900	-	X	-	-
3	CIT	4-X	900	-	X	-	-
3	CIT	5-X	900	-	X	-	-
3	CIT	6-X	900	-	X	-	-
3	CIT	7-X	900	-	X	-	-
3	CIT	8-X	900	-	X	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 78360 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 Ribonuclease pancreatic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1-X	126	996	600	189	194	13	0	0	0
1	2-X	126	996	600	189	194	13	0	0	0
1	3-X	126	996	600	189	194	13	0	0	0
1	4-X	126	996	600	189	194	13	0	0	0
1	5-X	126	996	600	189	194	13	0	0	0
1	6-X	126	996	600	189	194	13	0	0	0
1	7-X	126	996	600	189	194	13	0	0	0
1	8-X	126	996	600	189	194	13	0	0	0
1	1-Z	126	996	600	189	194	13	0	0	0
1	2-Z	126	996	600	189	194	13	0	0	0
1	3-Z	126	996	600	189	194	13	0	0	0
1	4-Z	126	996	600	189	194	13	0	0	0
1	5-Z	126	996	600	189	194	13	0	0	0
1	6-Z	126	996	600	189	194	13	0	0	0
1	7-Z	126	996	600	189	194	13	0	0	0
1	8-Z	126	996	600	189	194	13	0	0	0

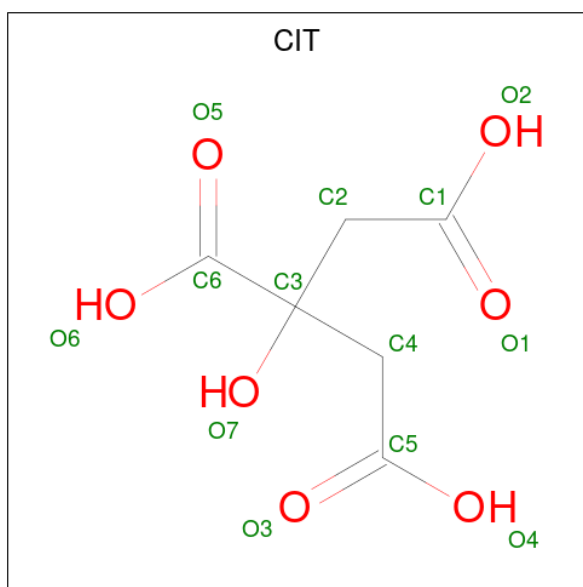
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	0	MET	-	initiating methionine	UNP P07998
Z	0	MET	-	initiating methionine	UNP P07998

- Molecule 2 is a protein called Ribonuclease inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-W	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	2-W	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	3-W	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	4-W	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	5-W	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	6-W	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	7-W	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	8-W	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	1-Y	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	2-Y	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	3-Y	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	4-Y	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	5-Y	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	6-Y	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	7-Y	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			
2	8-Y	460	Total	C	N	O	S	0	0	0
			3468	2142	605	687	34			

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-X	1	Total C O 13 6 7	0	0
3	2-X	1	Total C O 13 6 7	0	0
3	3-X	1	Total C O 13 6 7	0	0
3	4-X	1	Total C O 13 6 7	0	0
3	5-X	1	Total C O 13 6 7	0	0
3	6-X	1	Total C O 13 6 7	0	0
3	7-X	1	Total C O 13 6 7	0	0
3	8-X	1	Total C O 13 6 7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-X	103	Total O 103 103	0	0
4	2-X	107	Total O 107 107	0	0
4	3-X	108	Total O 108 108	0	0
4	4-X	107	Total O 107 107	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	5-X	111	Total 111	O 111	0	0
4	6-X	109	Total 109	O 109	0	0
4	7-X	111	Total 111	O 111	0	0
4	8-X	106	Total 106	O 106	0	0
4	1-W	300	Total 300	O 300	0	0
4	2-W	304	Total 304	O 304	0	0
4	3-W	298	Total 298	O 298	0	0
4	4-W	298	Total 298	O 298	0	0
4	5-W	298	Total 298	O 298	0	0
4	6-W	299	Total 299	O 299	0	0
4	7-W	298	Total 298	O 298	0	0
4	8-W	305	Total 305	O 305	0	0
4	1-Z	134	Total 134	O 134	0	0
4	2-Z	134	Total 134	O 134	0	0
4	3-Z	135	Total 135	O 135	0	0
4	4-Z	133	Total 133	O 133	0	0
4	5-Z	132	Total 132	O 132	0	0
4	6-Z	127	Total 127	O 127	0	0
4	7-Z	132	Total 132	O 132	0	0
4	8-Z	131	Total 131	O 131	0	0
4	1-Y	317	Total 317	O 317	0	0

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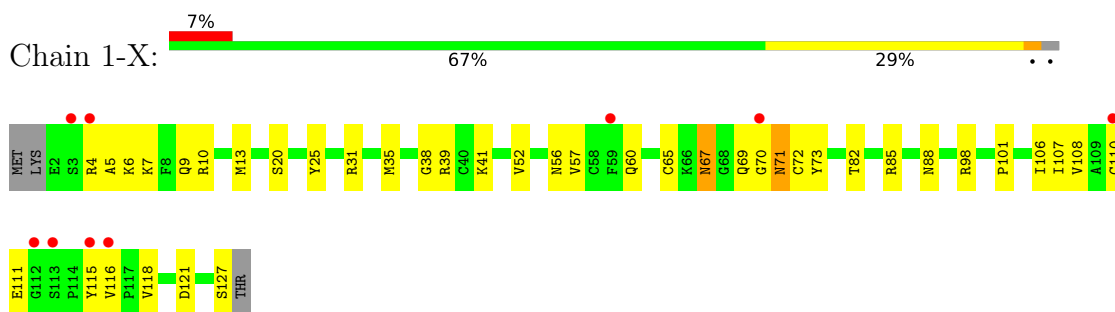
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	2-Y	309	Total 309	O 309	0	0
4	3-Y	313	Total 313	O 313	0	0
4	4-Y	316	Total 316	O 316	0	0
4	5-Y	313	Total 313	O 313	0	0
4	6-Y	319	Total 319	O 319	0	0
4	7-Y	313	Total 313	O 313	0	0
4	8-Y	312	Total 312	O 312	0	0

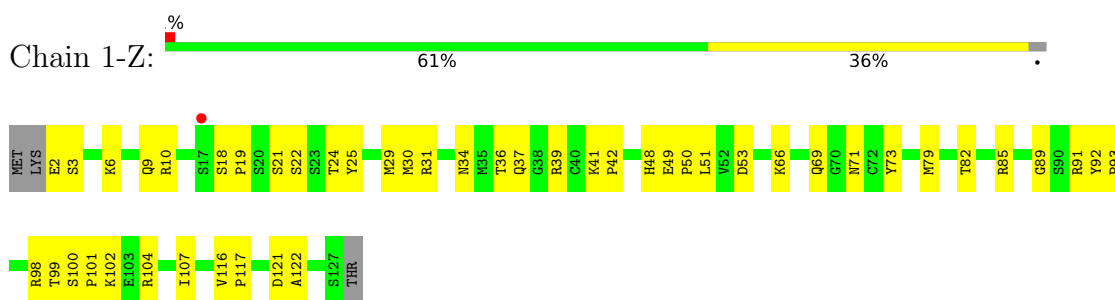
### 3 Residue-property plots [i](#)

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.

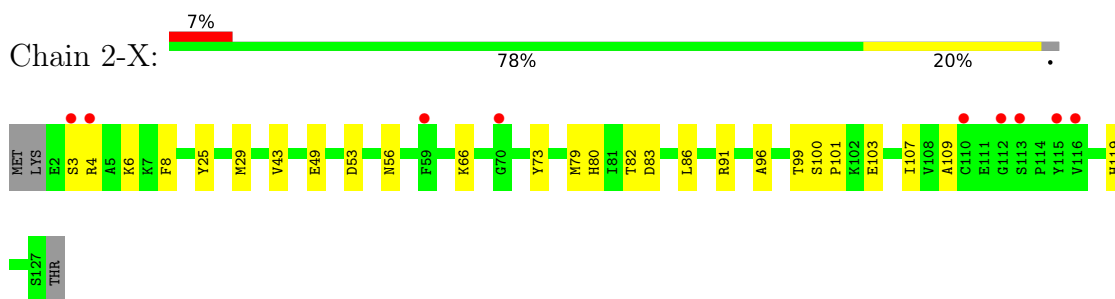
- Molecule 1: Ribonuclease pancreatic



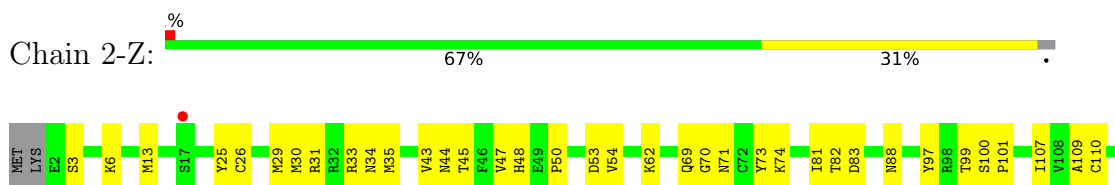
- Molecule 1: Ribonuclease pancreatic



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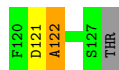
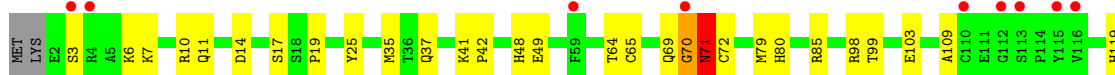
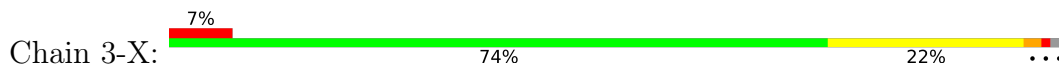


- Molecule 1: Ribonuclease pancreatic

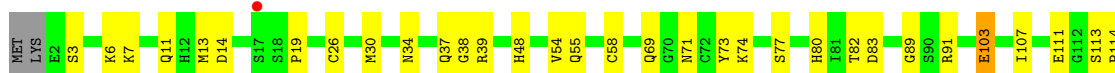




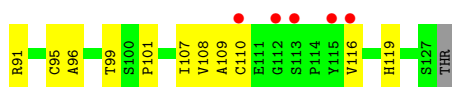
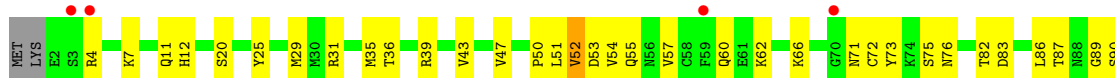
- Molecule 1: Ribonuclease pancreatic



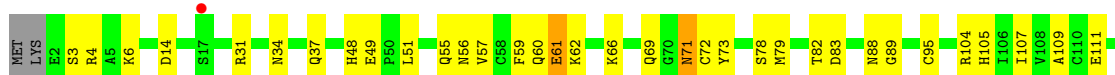
- Molecule 1: Ribonuclease pancreatic



- Molecule 1: Ribonuclease pancreatic



- Molecule 1: Ribonuclease pancreatic



- Molecule 1: Ribonuclease pancreatic

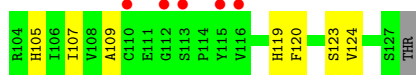




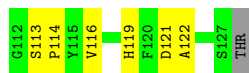
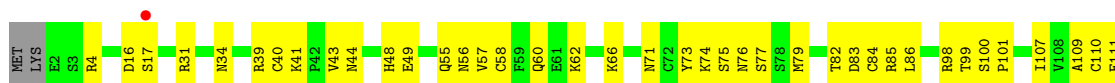
- Molecule 1: Ribonuclease pancreatic



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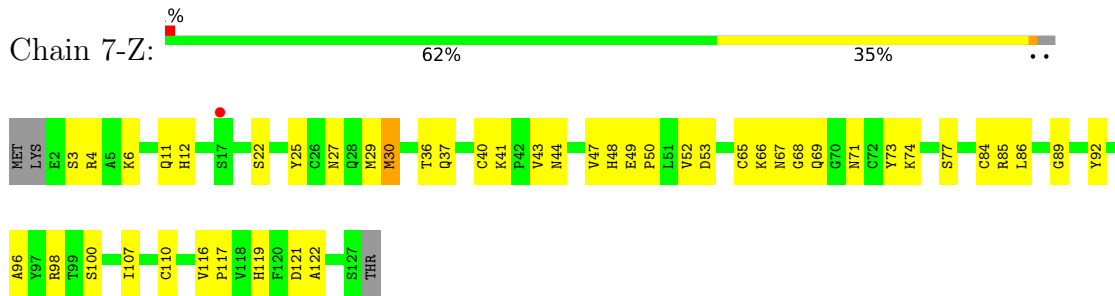
- Molecule 1: Ribonuclease pancreatic



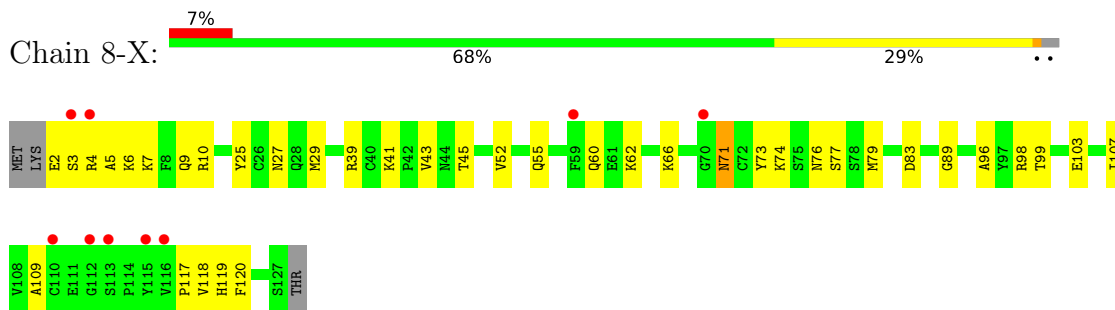
- Molecule 1: Ribonuclease pancreatic



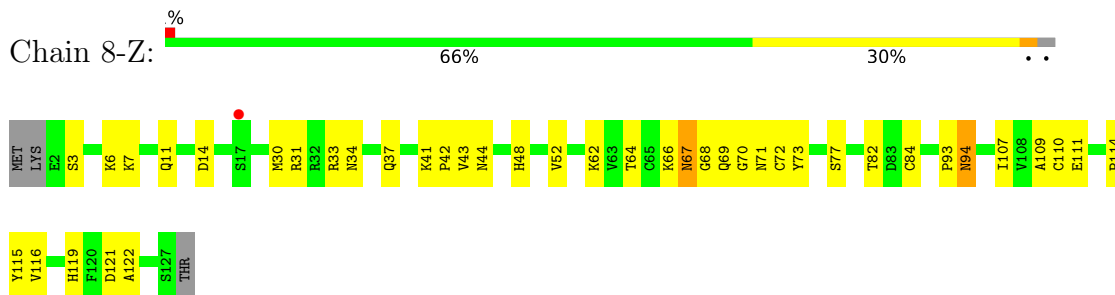
• Molecule 1: Ribonuclease pancreatic



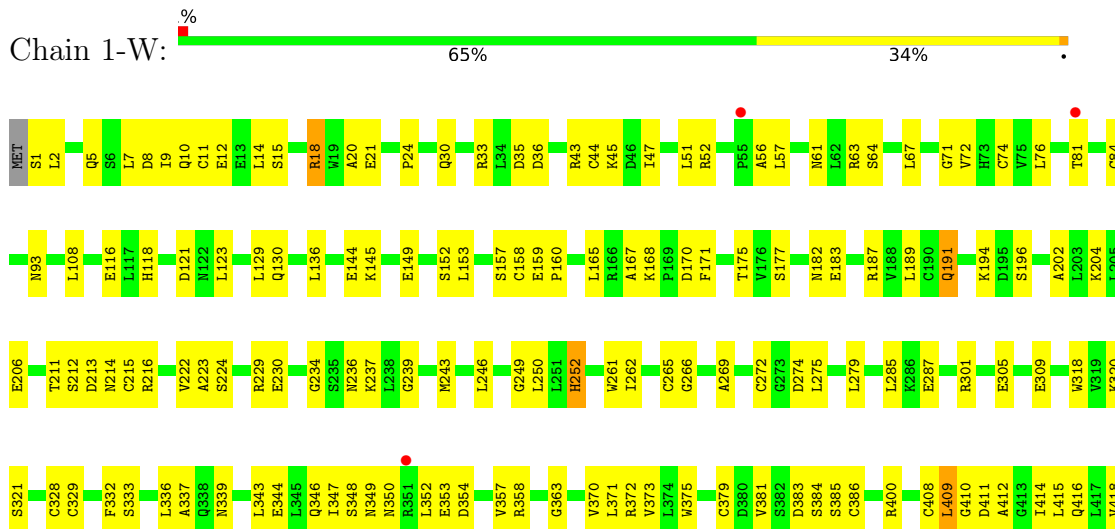
• Molecule 1: Ribonuclease pancreatic



• Molecule 1: Ribonuclease pancreatic

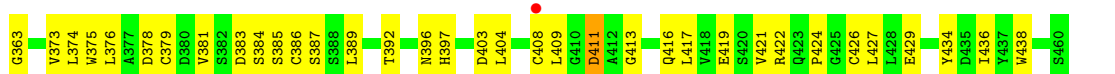
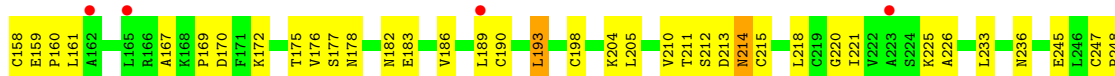
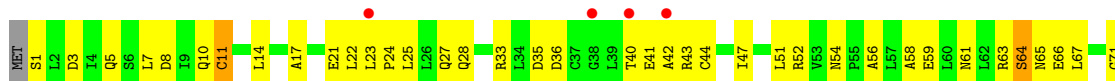


• Molecule 2: Ribonuclease inhibitor

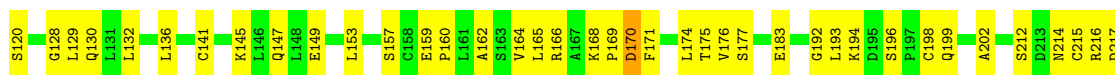
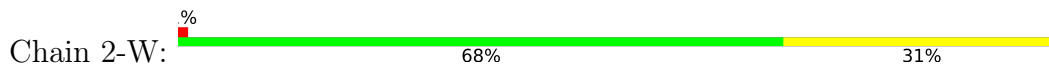




• Molecule 2: Ribonuclease inhibitor



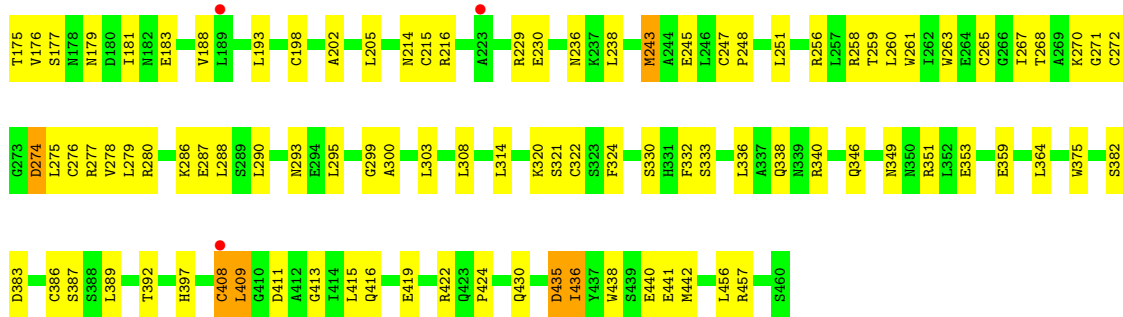
• Molecule 2: Ribonuclease inhibitor



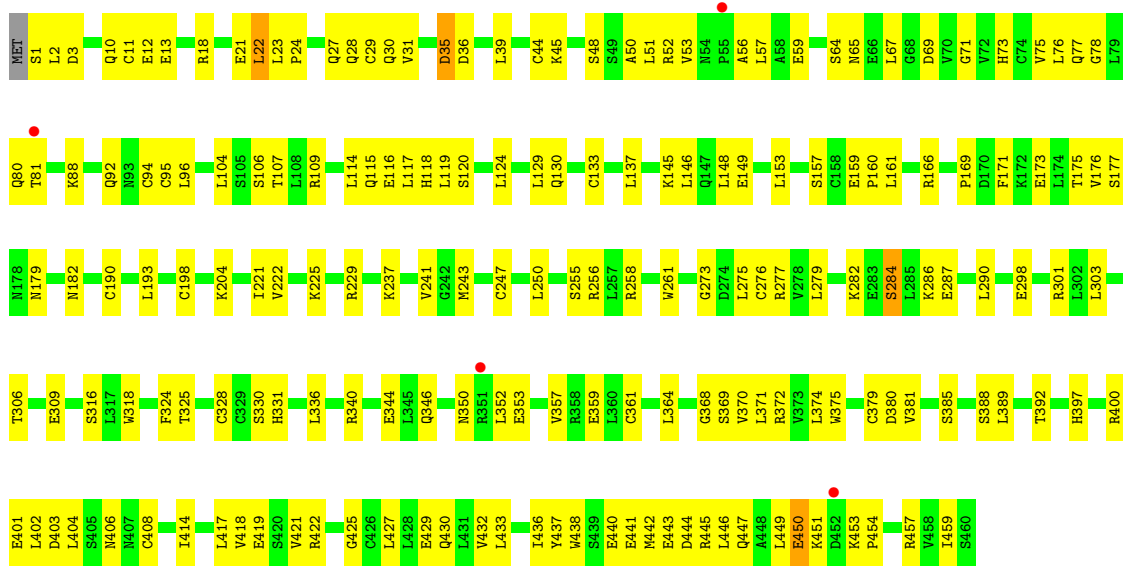
• Molecule 2: Ribonuclease inhibitor



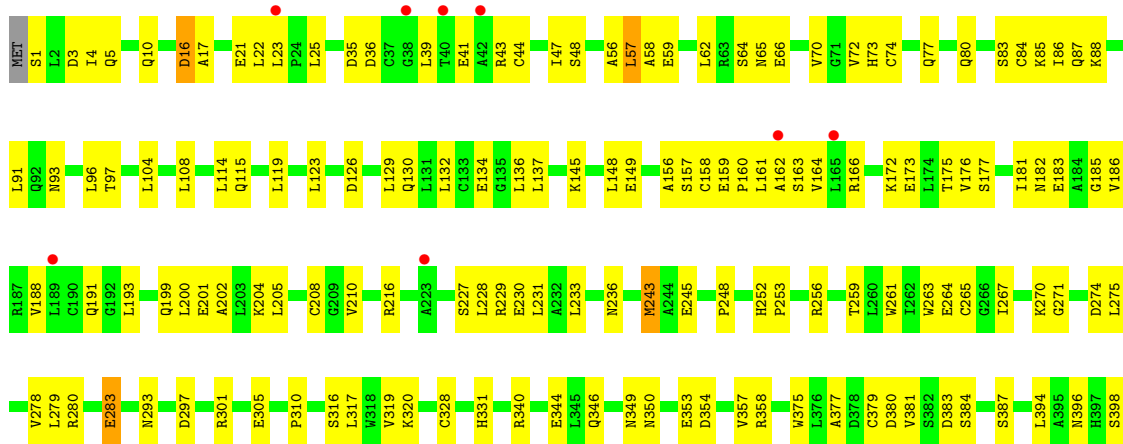




• Molecule 2: Ribonuclease inhibitor



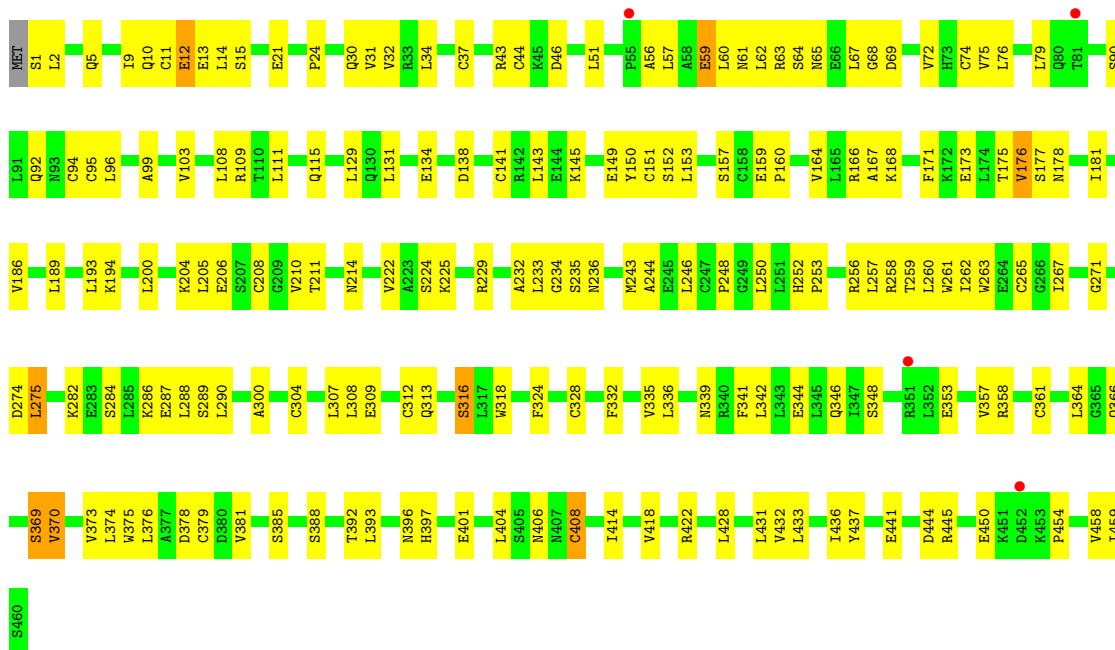
• Molecule 2: Ribonuclease inhibitor



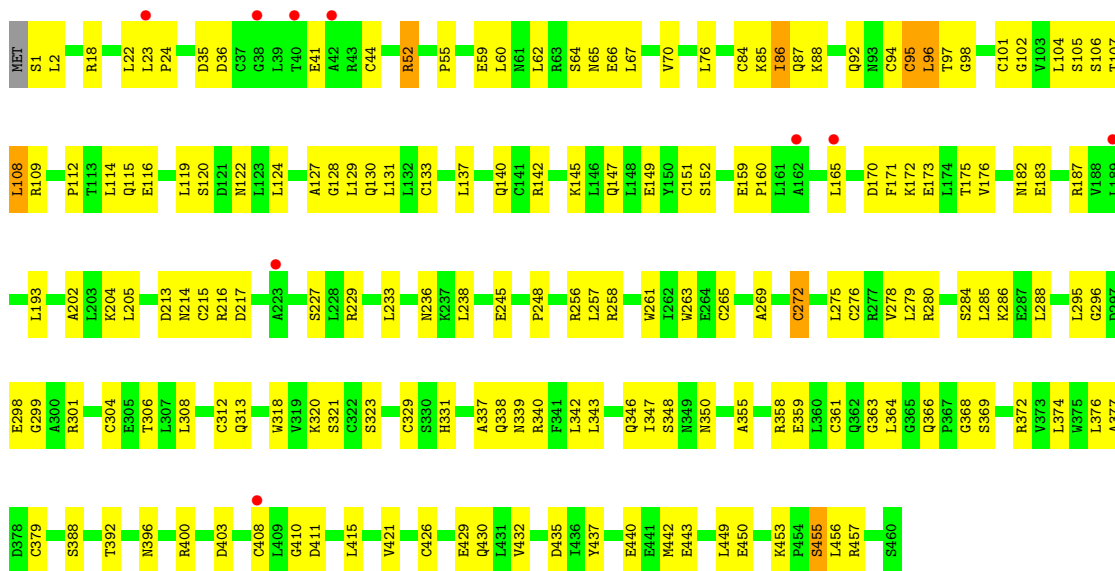




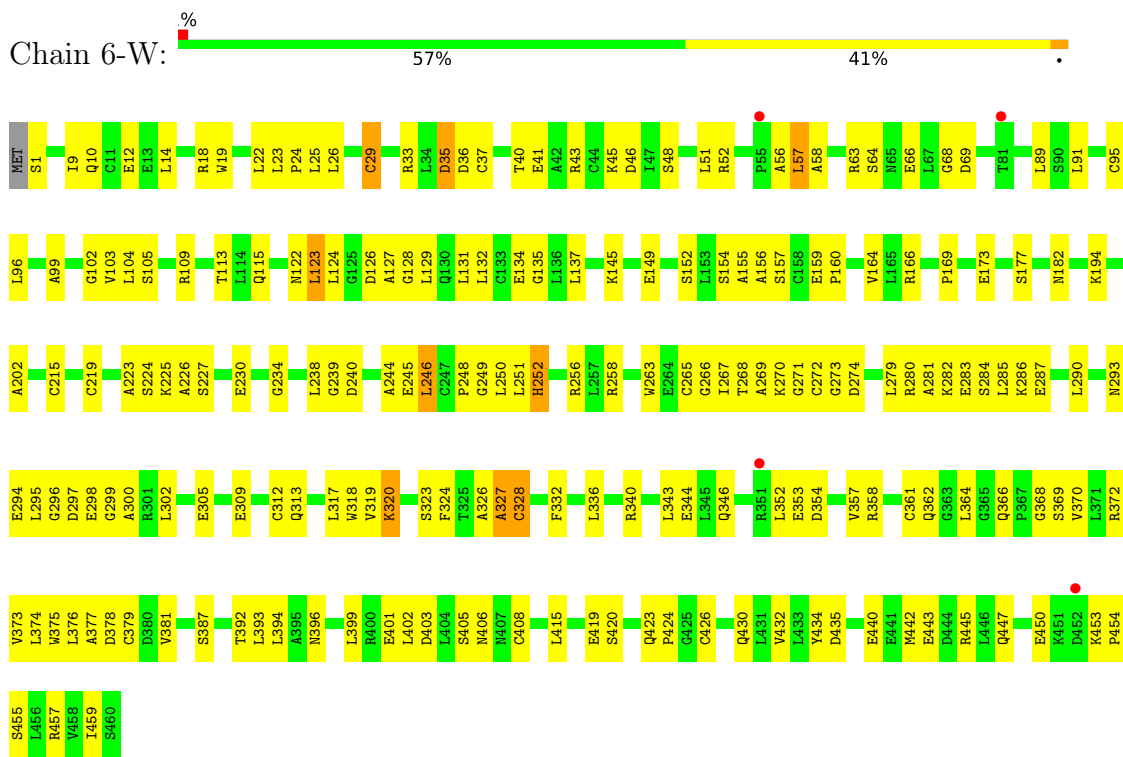
• Molecule 2: Ribonuclease inhibitor



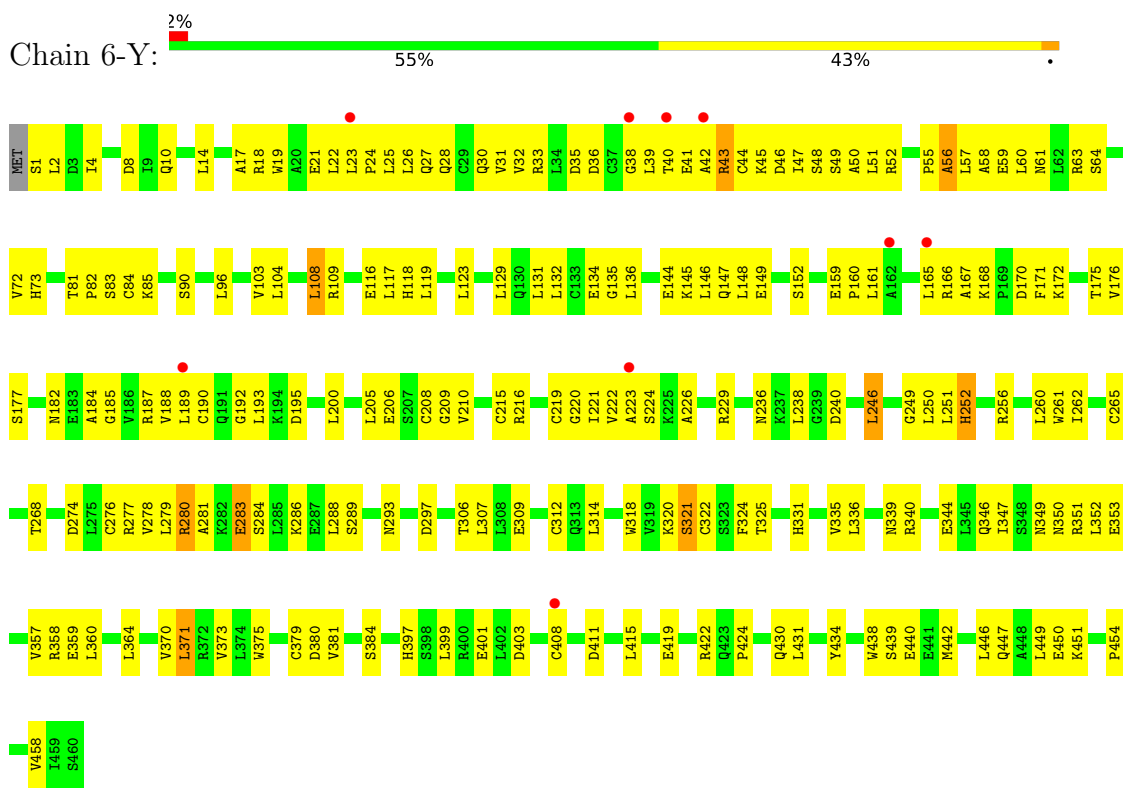
• Molecule 2: Ribonuclease inhibitor



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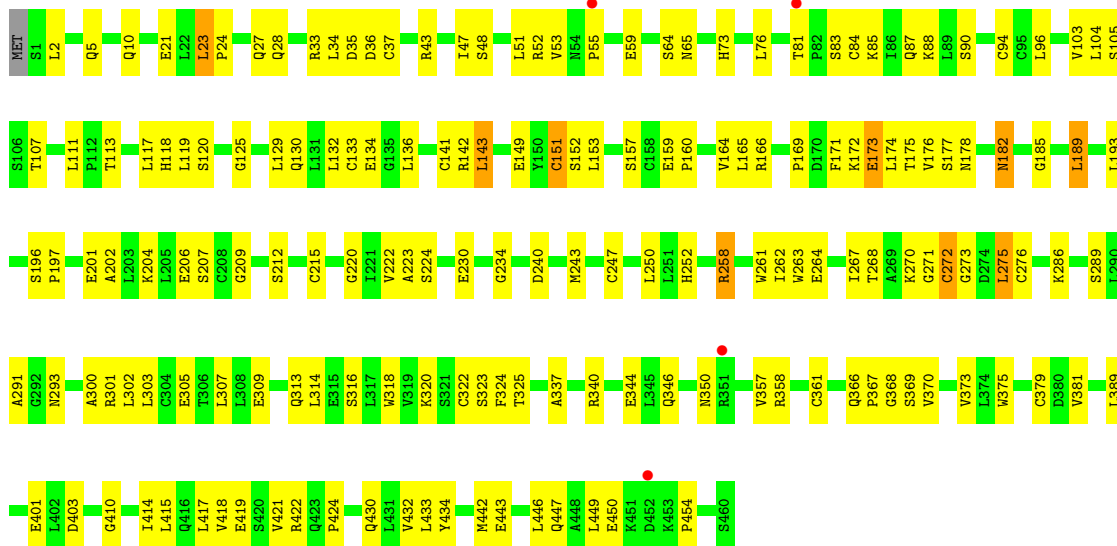


• Molecule 2: Ribonuclease inhibitor

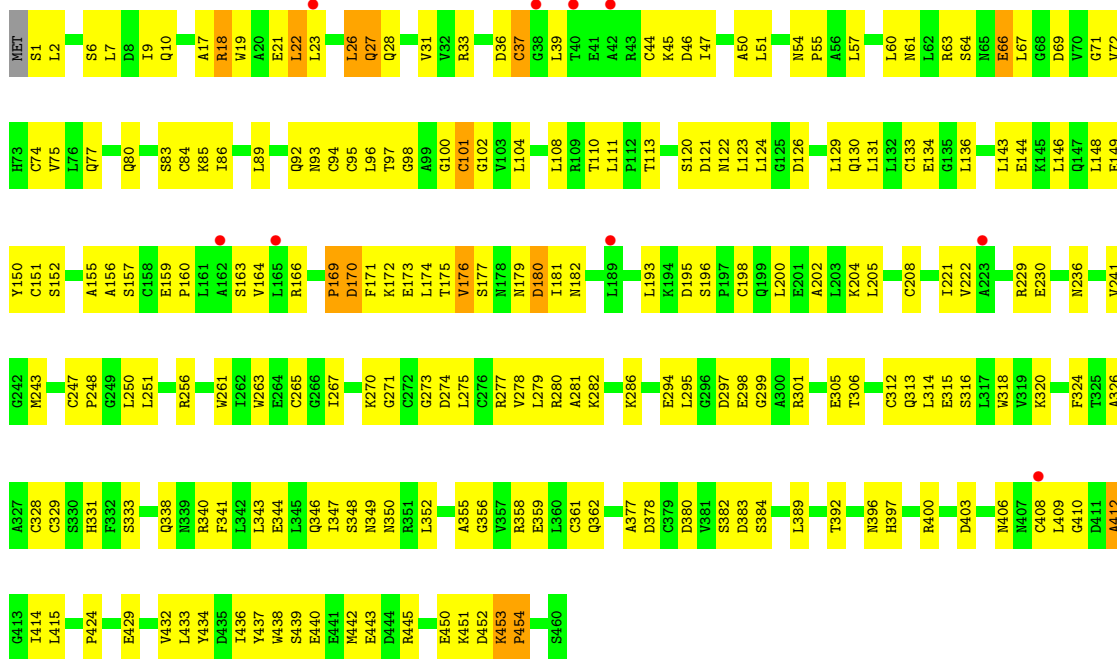


• Molecule 2: Ribonuclease inhibitor

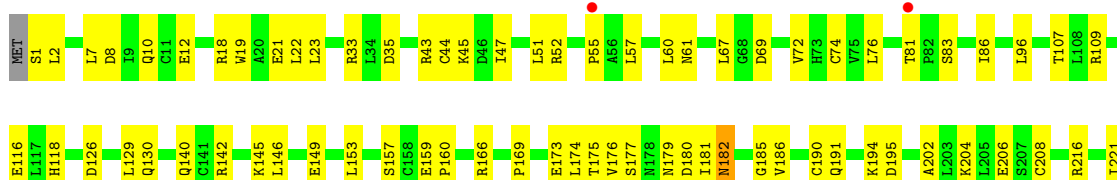
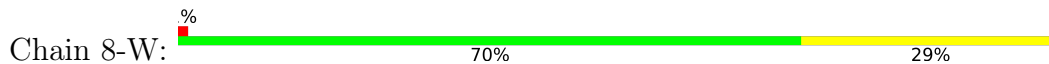




• Molecule 2: Ribonuclease inhibitor

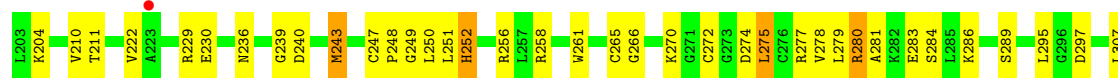
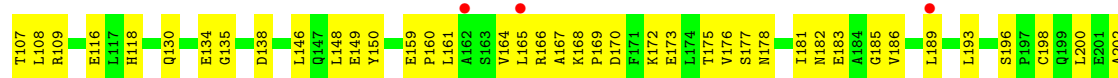


• Molecule 2: Ribonuclease inhibitor





● Molecule 2: Ribonuclease inhibitor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.34Å 107.55Å 155.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.17 – 1.95 47.17 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.8 (47.17-1.95) 96.9 (47.17-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 1.95Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.161 , 0.224 0.164 , 0.225	Depositor DCC
$R_{free}$ test set	4225 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	78360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIT

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	1-X	0.40	0/1016	0.65	0/1368
1	1-Z	0.46	0/1016	0.69	0/1368
1	2-X	0.41	0/1016	0.65	0/1368
1	2-Z	0.45	0/1016	0.68	0/1368
1	3-X	0.41	0/1016	0.66	0/1368
1	3-Z	0.44	0/1016	0.68	0/1368
1	4-X	0.42	0/1016	0.66	0/1368
1	4-Z	0.45	0/1016	0.68	0/1368
1	5-X	0.45	0/1016	0.68	0/1368
1	5-Z	0.47	0/1016	0.71	0/1368
1	6-X	0.43	0/1016	0.72	1/1368 (0.1%)
1	6-Z	0.48	0/1016	0.73	0/1368
1	7-X	0.44	0/1016	0.70	0/1368
1	7-Z	0.48	0/1016	0.72	0/1368
1	8-X	0.45	0/1016	0.70	0/1368
1	8-Z	0.50	0/1016	0.74	0/1368
2	1-W	0.42	0/3505	0.60	0/4744
2	1-Y	0.42	0/3505	0.62	0/4744
2	2-W	0.42	0/3505	0.60	0/4744
2	2-Y	0.41	0/3505	0.62	0/4744
2	3-W	0.42	0/3505	0.60	0/4744
2	3-Y	0.42	1/3505 (0.0%)	0.62	0/4744
2	4-W	0.41	0/3505	0.60	0/4744
2	4-Y	0.40	0/3505	0.63	0/4744
2	5-W	0.46	0/3505	0.65	0/4744
2	5-Y	0.45	0/3505	0.64	0/4744
2	6-W	0.45	0/3505	0.66	0/4744
2	6-Y	0.45	0/3505	0.65	0/4744
2	7-W	0.44	0/3505	0.64	0/4744
2	7-Y	0.44	1/3505 (0.0%)	0.65	0/4744
2	8-W	0.44	0/3505	0.63	0/4744
2	8-Y	0.43	0/3505	0.64	1/4744 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.43	2/72336 (0.0%)	0.64	2/97792 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3-Y	408	CYS	CB-SG	-6.10	1.71	1.82
2	7-Y	37	CYS	CB-SG	-5.23	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-Y	275	LEU	CA-CB-CG	5.50	127.94	115.30
1	6-X	40	CYS	CA-CB-SG	5.00	123.01	114.00

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	1-X	996	0	941	45	0
1	1-Z	996	0	941	47	0
1	2-X	996	0	941	17	0
1	2-Z	996	0	941	37	0
1	3-X	996	0	941	30	0
1	3-Z	996	0	941	31	0
1	4-X	996	0	941	45	0
1	4-Z	996	0	941	46	0
1	5-X	996	0	941	53	0
1	5-Z	996	0	941	50	0
1	6-X	996	0	941	41	0
1	6-Z	996	0	941	38	0
1	7-X	996	0	941	43	0
1	7-Z	996	0	941	41	0
1	8-X	996	0	941	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	8-Z	996	0	941	43	0
2	1-W	3468	0	3509	150	0
2	1-Y	3468	0	3509	172	0
2	2-W	3468	0	3509	135	0
2	2-Y	3468	0	3509	132	0
2	3-W	3468	0	3509	164	0
2	3-Y	3468	0	3509	160	0
2	4-W	3468	0	3509	172	0
2	4-Y	3468	0	3509	153	0
2	5-W	3468	0	3509	173	0
2	5-Y	3468	0	3509	161	0
2	6-W	3468	0	3509	191	0
2	6-Y	3468	0	3509	209	0
2	7-W	3468	0	3509	161	0
2	7-Y	3468	0	3509	218	0
2	8-W	3468	0	3509	136	0
2	8-Y	3468	0	3509	128	0
3	1-X	13	0	5	0	0
3	2-X	13	0	5	1	0
3	3-X	13	0	5	1	0
3	4-X	13	0	5	1	0
3	5-X	13	0	5	3	0
3	6-X	13	0	5	2	0
3	7-X	13	0	5	0	0
3	8-X	13	0	5	2	0
4	1-W	300	0	0	19	0
4	1-X	103	0	0	5	0
4	1-Y	317	0	0	25	0
4	1-Z	134	0	0	6	0
4	2-W	304	0	0	14	0
4	2-X	107	0	0	1	0
4	2-Y	309	0	0	7	0
4	2-Z	134	0	0	5	0
4	3-W	298	0	0	20	0
4	3-X	108	0	0	1	0
4	3-Y	313	0	0	22	0
4	3-Z	135	0	0	7	0
4	4-W	298	0	0	15	0
4	4-X	107	0	0	7	0
4	4-Y	316	0	0	24	0
4	4-Z	133	0	0	5	0
4	5-W	298	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	5-X	111	0	0	9	0
4	5-Y	313	0	0	17	0
4	5-Z	132	0	0	9	0
4	6-W	299	0	0	28	0
4	6-X	109	0	0	5	0
4	6-Y	319	0	0	39	0
4	6-Z	127	0	0	7	0
4	7-W	298	0	0	16	0
4	7-X	111	0	0	10	0
4	7-Y	313	0	0	28	0
4	7-Z	132	0	0	7	0
4	8-W	305	0	0	21	0
4	8-X	106	0	0	5	0
4	8-Y	312	0	0	17	0
4	8-Z	131	0	0	11	0
All	All	78360	0	71240	3062	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 21.

The worst 5 of 3062 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:Z:64:THR:HA	1:Z:70:GLY:HA2	1.19	1.12
2:Y:394:LEU:HD11	2:Y:423:GLN:HE22	1.19	1.08
1:X:64:THR:HA	1:X:70:GLY:HA2	1.32	1.07
2:W:55:PRO:HB3	2:W:83:SER:HB2	1.11	1.07
1:X:67:ASN:HD21	1:X:69:GLN:HG2	1.18	1.07

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 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	1-X	124/129 (96%)	109 (88%)	11 (9%)	4 (3%)	4	0
1	1-Z	124/129 (96%)	108 (87%)	16 (13%)	0	100	100
1	2-X	124/129 (96%)	119 (96%)	5 (4%)	0	100	100
1	2-Z	124/129 (96%)	116 (94%)	8 (6%)	0	100	100
1	3-X	124/129 (96%)	113 (91%)	8 (6%)	3 (2%)	6	1
1	3-Z	124/129 (96%)	116 (94%)	8 (6%)	0	100	100
1	4-X	124/129 (96%)	111 (90%)	12 (10%)	1 (1%)	19	9
1	4-Z	124/129 (96%)	112 (90%)	10 (8%)	2 (2%)	9	2
1	5-X	124/129 (96%)	105 (85%)	18 (14%)	1 (1%)	19	9
1	5-Z	124/129 (96%)	115 (93%)	8 (6%)	1 (1%)	19	9
1	6-X	124/129 (96%)	110 (89%)	12 (10%)	2 (2%)	9	2
1	6-Z	124/129 (96%)	117 (94%)	7 (6%)	0	100	100
1	7-X	124/129 (96%)	114 (92%)	10 (8%)	0	100	100
1	7-Z	124/129 (96%)	112 (90%)	11 (9%)	1 (1%)	19	9
1	8-X	124/129 (96%)	115 (93%)	8 (6%)	1 (1%)	19	9
1	8-Z	124/129 (96%)	110 (89%)	11 (9%)	3 (2%)	6	1
2	1-W	458/461 (99%)	421 (92%)	33 (7%)	4 (1%)	17	8
2	1-Y	458/461 (99%)	419 (92%)	30 (7%)	9 (2%)	7	1
2	2-W	458/461 (99%)	436 (95%)	22 (5%)	0	100	100
2	2-Y	458/461 (99%)	431 (94%)	24 (5%)	3 (1%)	22	11
2	3-W	458/461 (99%)	416 (91%)	38 (8%)	4 (1%)	17	8
2	3-Y	458/461 (99%)	423 (92%)	31 (7%)	4 (1%)	17	8
2	4-W	458/461 (99%)	420 (92%)	34 (7%)	4 (1%)	17	8
2	4-Y	458/461 (99%)	431 (94%)	24 (5%)	3 (1%)	22	11
2	5-W	458/461 (99%)	427 (93%)	27 (6%)	4 (1%)	17	8
2	5-Y	458/461 (99%)	424 (93%)	31 (7%)	3 (1%)	22	11
2	6-W	458/461 (99%)	414 (90%)	37 (8%)	7 (2%)	10	3
2	6-Y	458/461 (99%)	422 (92%)	31 (7%)	5 (1%)	14	5
2	7-W	458/461 (99%)	425 (93%)	31 (7%)	2 (0%)	34	22
2	7-Y	458/461 (99%)	411 (90%)	37 (8%)	10 (2%)	6	1
2	8-W	458/461 (99%)	422 (92%)	35 (8%)	1 (0%)	47	38
2	8-Y	458/461 (99%)	428 (93%)	26 (6%)	4 (1%)	17	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9312/9440 (99%)	8572 (92%)	654 (7%)	86 (1%)	17 8

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-X	71	ASN
2	1-W	409	LEU
2	1-Y	56	ALA
2	1-Y	310	PRO
2	1-Y	351	ARG

### 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	1-X	117/120 (98%)	114 (97%)	3 (3%)	46 36
1	1-Z	117/120 (98%)	115 (98%)	2 (2%)	60 55
1	2-X	117/120 (98%)	116 (99%)	1 (1%)	78 77
1	2-Z	117/120 (98%)	117 (100%)	0	100 100
1	3-X	117/120 (98%)	115 (98%)	2 (2%)	60 55
1	3-Z	117/120 (98%)	115 (98%)	2 (2%)	60 55
1	4-X	117/120 (98%)	115 (98%)	2 (2%)	60 55
1	4-Z	117/120 (98%)	116 (99%)	1 (1%)	78 77
1	5-X	117/120 (98%)	114 (97%)	3 (3%)	46 36
1	5-Z	117/120 (98%)	116 (99%)	1 (1%)	78 77
1	6-X	117/120 (98%)	116 (99%)	1 (1%)	78 77
1	6-Z	117/120 (98%)	117 (100%)	0	100 100
1	7-X	117/120 (98%)	115 (98%)	2 (2%)	60 55
1	7-Z	117/120 (98%)	116 (99%)	1 (1%)	78 77
1	8-X	117/120 (98%)	115 (98%)	2 (2%)	60 55
1	8-Z	117/120 (98%)	114 (97%)	3 (3%)	46 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1-W	396/397 (100%)	386 (98%)	10 (2%)	47	38
2	1-Y	396/397 (100%)	390 (98%)	6 (2%)	65	60
2	2-W	396/397 (100%)	390 (98%)	6 (2%)	65	60
2	2-Y	396/397 (100%)	391 (99%)	5 (1%)	69	65
2	3-W	396/397 (100%)	389 (98%)	7 (2%)	59	53
2	3-Y	396/397 (100%)	390 (98%)	6 (2%)	65	60
2	4-W	396/397 (100%)	389 (98%)	7 (2%)	59	53
2	4-Y	396/397 (100%)	390 (98%)	6 (2%)	65	60
2	5-W	396/397 (100%)	386 (98%)	10 (2%)	47	38
2	5-Y	396/397 (100%)	388 (98%)	8 (2%)	55	48
2	6-W	396/397 (100%)	386 (98%)	10 (2%)	47	38
2	6-Y	396/397 (100%)	385 (97%)	11 (3%)	43	33
2	7-W	396/397 (100%)	384 (97%)	12 (3%)	41	30
2	7-Y	396/397 (100%)	386 (98%)	10 (2%)	47	38
2	8-W	396/397 (100%)	392 (99%)	4 (1%)	76	74
2	8-Y	396/397 (100%)	390 (98%)	6 (2%)	65	60
All	All	8208/8272 (99%)	8058 (98%)	150 (2%)	59	53

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	7-W	152	SER
1	8-Z	115	TYR
2	7-W	258	ARG
2	7-Y	150	TYR
2	3-Y	359	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
2	6-Y	338	GLN
1	8-Z	37	GLN
1	7-X	37	GLN
2	7-Y	77	GLN
2	8-Y	338	GLN

### 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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CIT	3-X	900	-	12,12,12	4.34	6 (50%)	17,17,17	5.76	10 (58%)
3	CIT	7-X	900	-	12,12,12	4.49	6 (50%)	17,17,17	5.72	10 (58%)
3	CIT	1-X	900	-	12,12,12	4.58	6 (50%)	17,17,17	6.07	11 (64%)
3	CIT	4-X	900	-	12,12,12	4.34	7 (58%)	17,17,17	5.73	9 (52%)
3	CIT	8-X	900	-	12,12,12	4.19	6 (50%)	17,17,17	5.80	11 (64%)
3	CIT	5-X	900	-	12,12,12	4.89	6 (50%)	17,17,17	5.72	10 (58%)
3	CIT	6-X	900	-	12,12,12	4.69	7 (58%)	17,17,17	5.64	10 (58%)
3	CIT	2-X	900	-	12,12,12	4.55	6 (50%)	17,17,17	5.70	10 (58%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIT	3-X	900	-	-	8/16/16/16	-
3	CIT	7-X	900	-	-	6/16/16/16	-
3	CIT	1-X	900	-	-	4/16/16/16	-
3	CIT	4-X	900	-	-	8/16/16/16	-
3	CIT	8-X	900	-	-	5/16/16/16	-
3	CIT	5-X	900	-	-	3/16/16/16	-
3	CIT	6-X	900	-	-	5/16/16/16	-
3	CIT	2-X	900	-	-	5/16/16/16	-

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-X	900	CIT	C3-C6	15.05	1.69	1.53
3	6-X	900	CIT	C3-C6	14.37	1.68	1.53
3	1-X	900	CIT	C3-C6	14.03	1.68	1.53
3	2-X	900	CIT	C3-C6	13.86	1.67	1.53
3	7-X	900	CIT	C3-C6	13.63	1.67	1.53

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-X	900	CIT	O7-C3-C6	-14.27	88.84	108.86
3	4-X	900	CIT	O7-C3-C6	-14.05	89.14	108.86
3	7-X	900	CIT	O7-C3-C6	-14.04	89.16	108.86
3	2-X	900	CIT	O7-C3-C6	-13.93	89.30	108.86
3	3-X	900	CIT	O7-C3-C6	-13.87	89.39	108.86

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	1-X	900	CIT	C1-C2-C3-O7
3	1-X	900	CIT	C2-C3-C4-C5
3	2-X	900	CIT	C1-C2-C3-O7
3	2-X	900	CIT	C2-C3-C4-C5
3	3-X	900	CIT	C1-C2-C3-O7

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	3-X	900	CIT	1	0
3	4-X	900	CIT	1	0
3	8-X	900	CIT	2	0
3	5-X	900	CIT	3	0
3	6-X	900	CIT	2	0
3	2-X	900	CIT	1	0

## 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	1-X	126/129 (97%)	0.18	9 (7%) 16 24	13, 22, 37, 41	126 (100%)
1	1-Z	126/129 (97%)	-0.15	1 (0%) 86 90	10, 19, 31, 38	126 (100%)
1	2-X	126/129 (97%)	0.18	9 (7%) 16 24	13, 22, 37, 41	126 (100%)
1	2-Z	126/129 (97%)	-0.15	1 (0%) 86 90	10, 19, 31, 38	126 (100%)
1	3-X	126/129 (97%)	0.18	9 (7%) 16 24	13, 22, 37, 41	126 (100%)
1	3-Z	126/129 (97%)	-0.15	1 (0%) 86 90	10, 19, 31, 38	126 (100%)
1	4-X	126/129 (97%)	0.18	9 (7%) 16 24	13, 22, 37, 41	126 (100%)
1	4-Z	126/129 (97%)	-0.15	1 (0%) 86 90	10, 19, 31, 38	126 (100%)
1	5-X	126/129 (97%)	0.18	9 (7%) 16 24	13, 22, 37, 41	126 (100%)
1	5-Z	126/129 (97%)	-0.15	1 (0%) 86 90	10, 19, 31, 38	126 (100%)
1	6-X	126/129 (97%)	0.18	9 (7%) 16 24	13, 22, 37, 41	126 (100%)
1	6-Z	126/129 (97%)	-0.15	1 (0%) 86 90	10, 19, 31, 38	126 (100%)
1	7-X	126/129 (97%)	0.18	9 (7%) 16 24	13, 22, 37, 41	126 (100%)
1	7-Z	126/129 (97%)	-0.15	1 (0%) 86 90	10, 19, 31, 38	126 (100%)
1	8-X	126/129 (97%)	0.18	9 (7%) 16 24	13, 22, 37, 41	126 (100%)
1	8-Z	126/129 (97%)	-0.15	1 (0%) 86 90	10, 19, 31, 38	126 (100%)
2	1-W	460/461 (99%)	-0.17	4 (0%) 84 89	11, 21, 32, 43	460 (100%)
2	1-Y	460/461 (99%)	-0.03	9 (1%) 65 73	8, 21, 34, 44	460 (100%)
2	2-W	460/461 (99%)	-0.17	4 (0%) 84 89	11, 21, 32, 43	460 (100%)
2	2-Y	460/461 (99%)	-0.03	9 (1%) 65 73	8, 21, 34, 44	460 (100%)
2	3-W	460/461 (99%)	-0.17	4 (0%) 84 89	11, 21, 32, 43	460 (100%)
2	3-Y	460/461 (99%)	-0.03	9 (1%) 65 73	8, 21, 34, 44	460 (100%)
2	4-W	460/461 (99%)	-0.17	4 (0%) 84 89	11, 21, 32, 43	460 (100%)
2	4-Y	460/461 (99%)	-0.03	9 (1%) 65 73	8, 21, 34, 44	460 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	5-W	460/461 (99%)	-0.17	4 (0%) 84 89	11, 21, 32, 43	460 (100%)
2	5-Y	460/461 (99%)	-0.03	9 (1%) 65 73	8, 21, 34, 44	460 (100%)
2	6-W	460/461 (99%)	-0.17	4 (0%) 84 89	11, 21, 32, 43	460 (100%)
2	6-Y	460/461 (99%)	-0.03	9 (1%) 65 73	8, 21, 34, 44	460 (100%)
2	7-W	460/461 (99%)	-0.17	4 (0%) 84 89	11, 21, 32, 43	460 (100%)
2	7-Y	460/461 (99%)	-0.03	9 (1%) 65 73	8, 21, 34, 44	460 (100%)
2	8-W	460/461 (99%)	-0.17	4 (0%) 84 89	11, 21, 32, 43	460 (100%)
2	8-Y	460/461 (99%)	-0.03	9 (1%) 65 73	8, 21, 34, 44	460 (100%)
All	All	9376/9440 (99%)	-0.08	184 (1%) 66 73	8, 21, 33, 44	9376 (100%)

The worst 5 of 184 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-X	112	GLY	4.6
1	2-X	112	GLY	4.6
1	3-X	112	GLY	4.6
1	4-X	112	GLY	4.6
1	5-X	112	GLY	4.6

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CIT	1-X	900	13/13	0.95	0.16	12,22,25,27	13
3	CIT	2-X	900	13/13	0.95	0.16	19,24,28,28	13

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CIT	3-X	900	13/13	0.95	0.16	21,24,29,31	13
3	CIT	4-X	900	13/13	0.95	0.16	18,26,29,30	13
3	CIT	5-X	900	13/13	0.95	0.16	10,18,22,26	13
3	CIT	6-X	900	13/13	0.95	0.16	18,24,26,27	13
3	CIT	7-X	900	13/13	0.95	0.16	20,24,28,29	13
3	CIT	8-X	900	13/13	0.95	0.16	1,25,30,32	13

## 6.5 Other polymers [i](#)

There are no such residues in this entry.