



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 07:23 PM UTC

PDB ID : 2Q4G / pdb_00002q4g
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

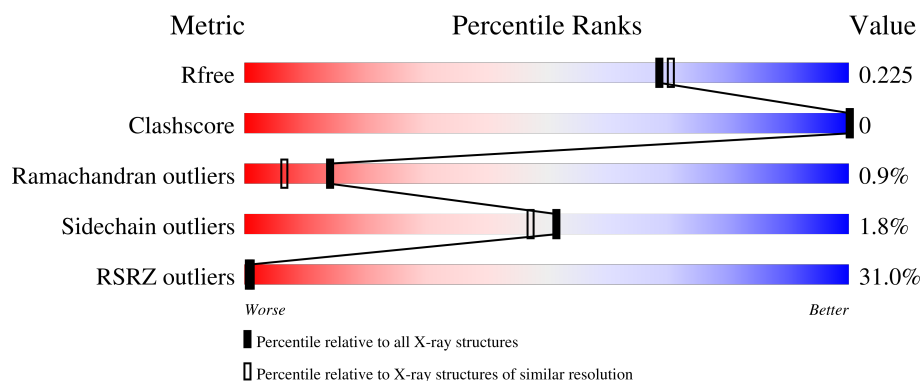
1 Overall quality at a glance

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.



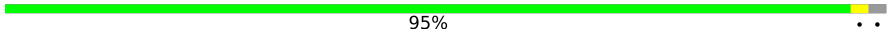
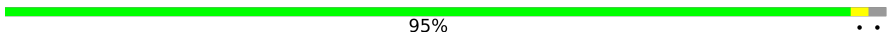
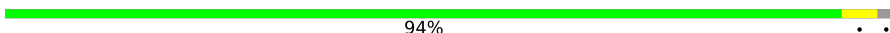
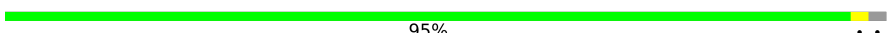
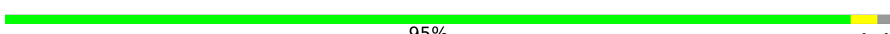
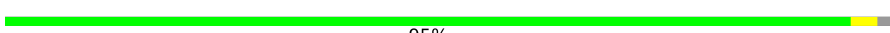
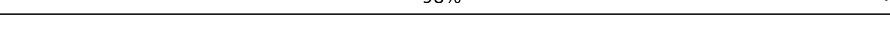
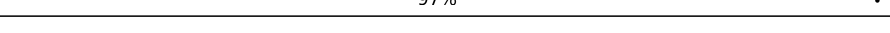
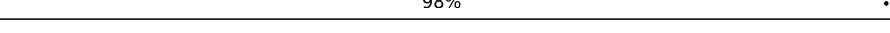
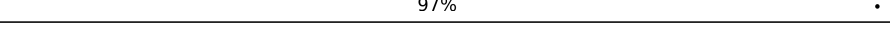
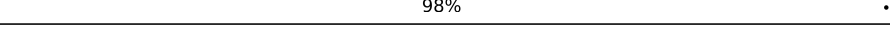
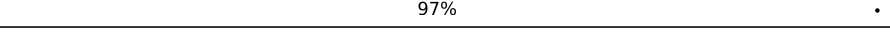
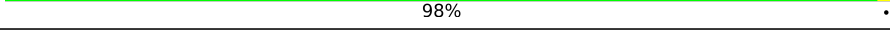
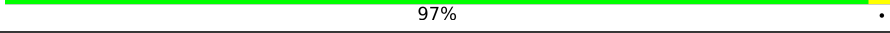
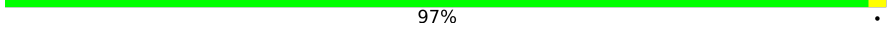
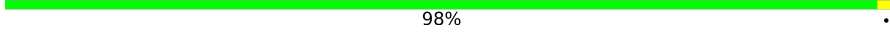
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 ≥ 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	33% 93% 5%
1	1-Z	129	29% 95% ..
1	2-X	129	96% ..
1	2-Z	129	95% ..
1	3-X	129	94% ..

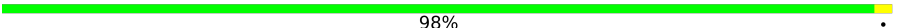
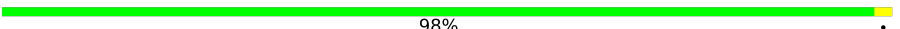
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Mol	Chain	Length	Quality of chain
1	3-Z	129	 95% ..
1	4-X	129	 95% ..
1	4-Z	129	 94% ..
1	5-X	129	 95% ..
1	5-Z	129	 95% ..
1	6-X	129	 95% ..
1	6-Z	129	 95% ..
1	7-X	129	 96% ..
1	7-Z	129	 95% ..
1	8-X	129	 95% ..
1	8-Z	129	 93% 5% .
2	1-W	461	 26% 97% .
2	1-Y	461	 35% 97% .
2	2-W	461	 98% .
2	2-Y	461	 98% .
2	3-W	461	 97% .
2	3-Y	461	 98% .
2	4-W	461	 97% .
2	4-Y	461	 98% .
2	5-W	461	 97% .
2	5-Y	461	 98% .
2	6-W	461	 97% .
2	6-Y	461	 97% .
2	7-W	461	 98% .
2	7-Y	461	 96% .

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Mol	Chain	Length	Quality of chain
2	8-W	461	 98%
2	8-Y	461	 98%

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

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
1	1-X	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	2-X	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	3-X	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	4-X	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	5-X	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	6-X	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	7-X	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	8-X	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	1-Z	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	2-Z	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	3-Z	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	4-Z	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	5-Z	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	6-Z	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	7-Z	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			
1	8-Z	126	Total	C	N	O	S	0	0	0
			996	600	189	194	13			

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 (CCD ID: CIT) (formula: C₆H₈O₇).



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

- Molecule 4 is water.

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

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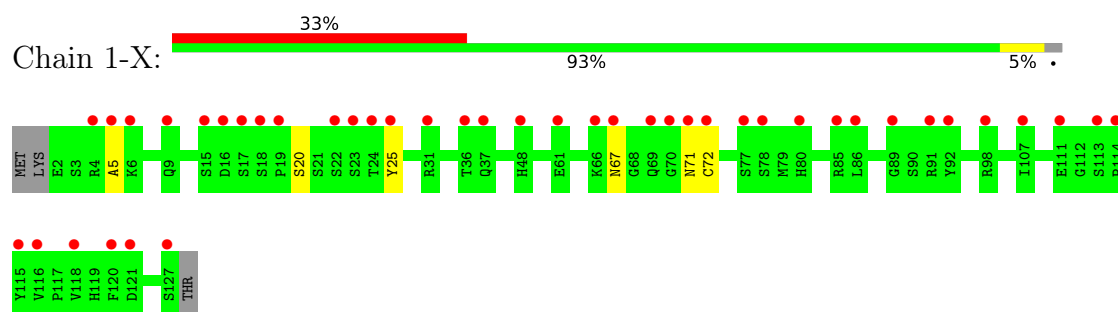
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	2-Y	309	Total 309	O 309	0	0
4	3-Y	313	Total 313	O 313	0	0
4	4-Y	316	Total 316	O 316	0	0
4	5-Y	313	Total 313	O 313	0	0
4	6-Y	319	Total 319	O 319	0	0
4	7-Y	313	Total 313	O 313	0	0
4	8-Y	312	Total 312	O 312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

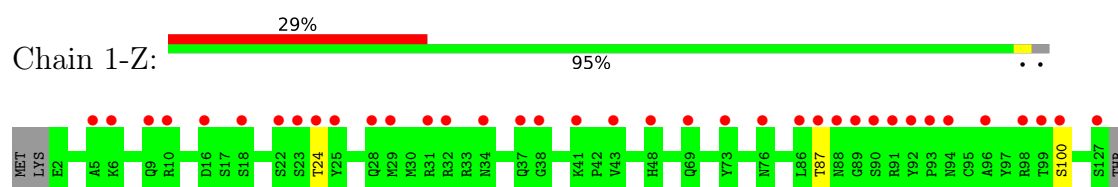
3 Residue-property plots [i](#)

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.

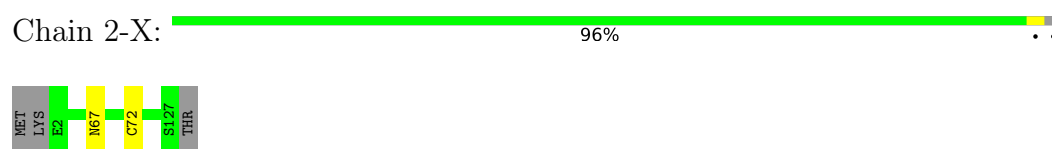
- Molecule 1: Ribonuclease pancreatic



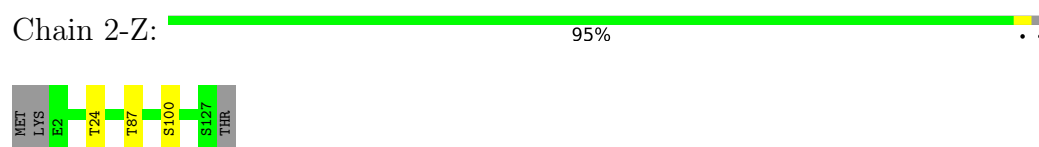
- Molecule 1: Ribonuclease pancreatic



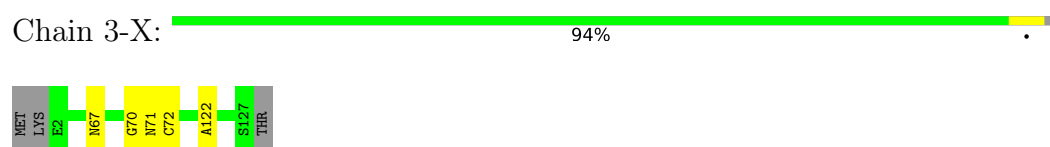
- Molecule 1: Ribonuclease pancreatic



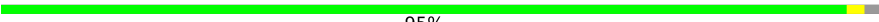
- Molecule 1: Ribonuclease pancreatic



- Molecule 1: Ribonuclease pancreatic

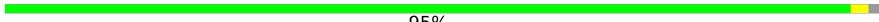


- Molecule 1: Ribonuclease pancreatic

Chain 3-Z:  95% ..



- Molecule 1: Ribonuclease pancreatic

Chain 4-X:  95% ..

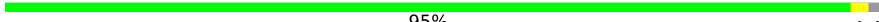


- Molecule 1: Ribonuclease pancreatic

Chain 4-Z:  94% ..

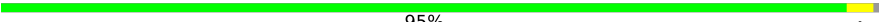


- Molecule 1: Ribonuclease pancreatic

Chain 5-X:  95% ..

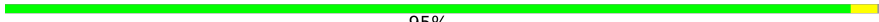


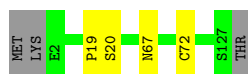
- Molecule 1: Ribonuclease pancreatic

Chain 5-Z:  95% ..

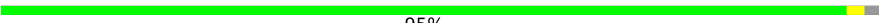


- Molecule 1: Ribonuclease pancreatic

Chain 6-X:  95% ..

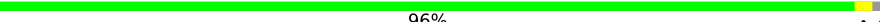


- Molecule 1: Ribonuclease pancreatic

Chain 6-Z:  95% ..

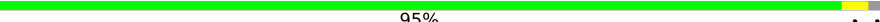


- Molecule 1: Ribonuclease pancreatic

Chain 7-X:  96% ..

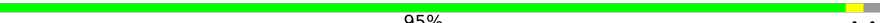


- Molecule 1: Ribonuclease pancreatic

Chain 7-Z:  95% ..



- Molecule 1: Ribonuclease pancreatic

Chain 8-X:  95% ..



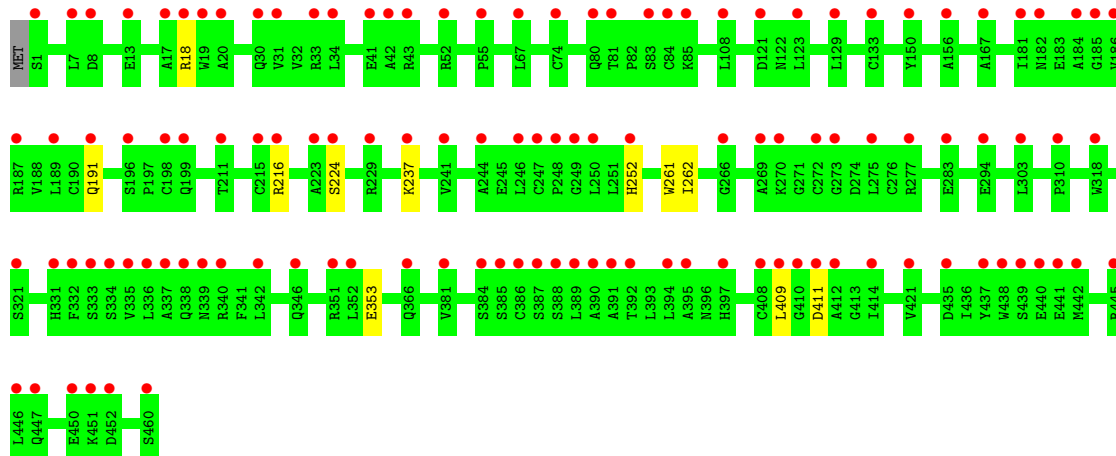
- Molecule 1: Ribonuclease pancreatic

Chain 8-Z:  93% 5% .

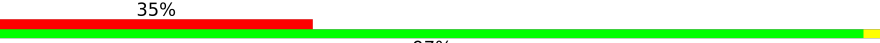


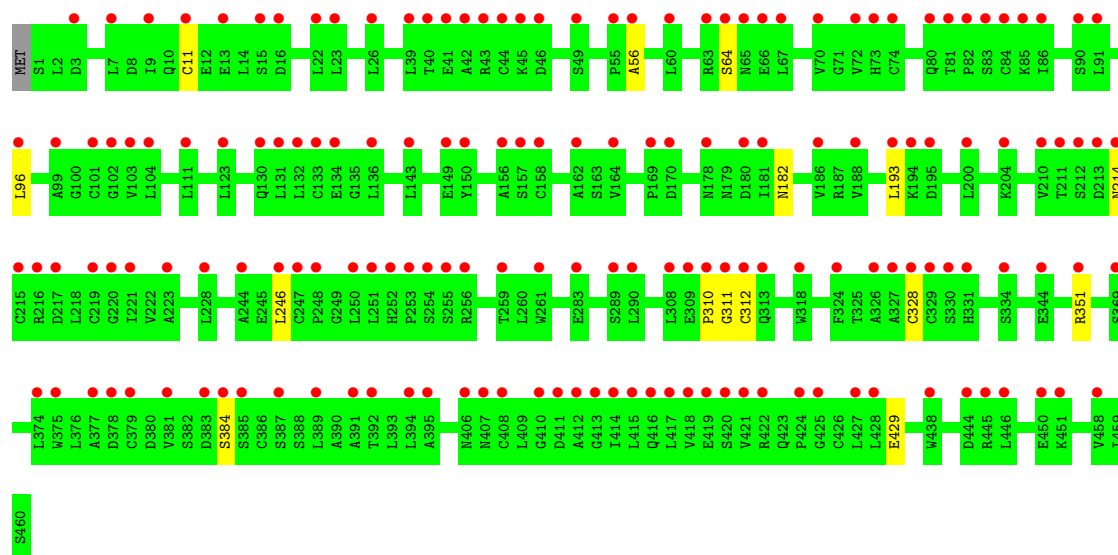
- Molecule 2: Ribonuclease inhibitor

Chain 1-W:  26% 97% .



- Molecule 2: Ribonuclease inhibitor

Chain 1-Y:  35% 97% .



- Molecule 2: Ribonuclease inhibitor

Chain 2-W: 98%



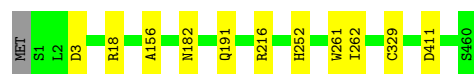
- Molecule 2: Ribonuclease inhibitor

Chain 2-Y: 98%



- Molecule 2: Ribonuclease inhibitor

Chain 3-W: 97%



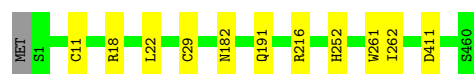
- Molecule 2: Ribonuclease inhibitor

Chain 3-Y: 98%

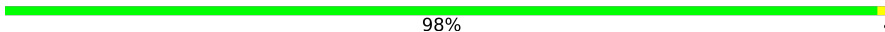


- Molecule 2: Ribonuclease inhibitor

Chain 4-W: 97%

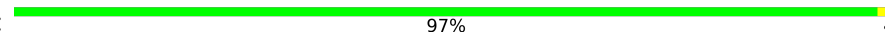


- Molecule 2: Ribonuclease inhibitor

Chain 4-Y:  98% .

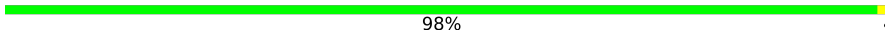


- Molecule 2: Ribonuclease inhibitor

Chain 5-W:  97% .

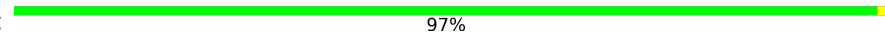


- Molecule 2: Ribonuclease inhibitor

Chain 5-Y:  98% .

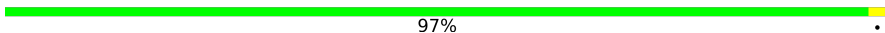


- Molecule 2: Ribonuclease inhibitor

Chain 6-W:  97% .

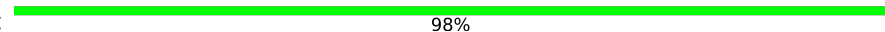


- Molecule 2: Ribonuclease inhibitor

Chain 6-Y:  97% .

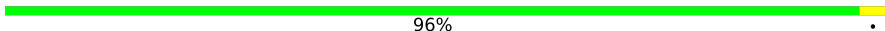


- Molecule 2: Ribonuclease inhibitor

Chain 7-W:  98% .

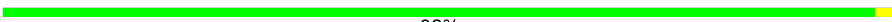


- Molecule 2: Ribonuclease inhibitor

Chain 7-Y:  96% .

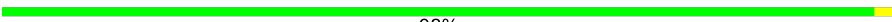


- Molecule 2: Ribonuclease inhibitor

Chain 8-W:  98% .



● Molecule 2: Ribonuclease inhibitor

Chain 8-Y:  98% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 1.95Å)	Xtriage
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 (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.04 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	78360	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage'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.*

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

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	0.28	0/1016	0.50	0/1368
1	1-Z	0.30	0/1016	0.49	0/1368
1	2-X	0.28	0/1016	0.50	0/1368
1	2-Z	0.30	0/1016	0.49	0/1368
1	3-X	0.28	0/1016	0.50	0/1368
1	3-Z	0.30	0/1016	0.49	0/1368
1	4-X	0.28	0/1016	0.50	0/1368
1	4-Z	0.30	0/1016	0.49	0/1368
1	5-X	0.28	0/1016	0.50	0/1368
1	5-Z	0.30	0/1016	0.49	0/1368
1	6-X	0.28	0/1016	0.50	0/1368
1	6-Z	0.30	0/1016	0.49	0/1368
1	7-X	0.28	0/1016	0.50	0/1368
1	7-Z	0.30	0/1016	0.49	0/1368
1	8-X	0.28	0/1016	0.50	0/1368
1	8-Z	0.30	0/1016	0.49	0/1368
2	1-W	0.28	0/3505	0.44	0/4744
2	1-Y	0.27	0/3505	0.44	0/4744
2	2-W	0.28	0/3505	0.44	0/4744
2	2-Y	0.27	0/3505	0.44	0/4744
2	3-W	0.28	0/3505	0.44	0/4744
2	3-Y	0.27	0/3505	0.44	0/4744
2	4-W	0.28	0/3505	0.44	0/4744
2	4-Y	0.27	0/3505	0.44	0/4744
2	5-W	0.28	0/3505	0.44	0/4744
2	5-Y	0.27	0/3505	0.44	0/4744
2	6-W	0.28	0/3505	0.44	0/4744
2	6-Y	0.27	0/3505	0.44	0/4744
2	7-W	0.28	0/3505	0.44	0/4744
2	7-Y	0.27	0/3505	0.44	0/4744
2	8-W	0.28	0/3505	0.44	0/4744
2	8-Y	0.27	0/3505	0.44	0/4744

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.28	0/72336	0.46	0/97792

There are no bond length outliers.

There are no bond angle outliers.

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	0	0
1	1-Z	996	0	941	0	0
1	2-X	996	0	941	0	0
1	2-Z	996	0	941	0	0
1	3-X	996	0	941	0	0
1	3-Z	996	0	941	0	0
1	4-X	996	0	941	0	0
1	4-Z	996	0	941	0	0
1	5-X	996	0	941	0	0
1	5-Z	996	0	941	0	0
1	6-X	996	0	941	0	0
1	6-Z	996	0	941	0	0
1	7-X	996	0	941	0	0
1	7-Z	996	0	941	0	0
1	8-X	996	0	941	0	0
1	8-Z	996	0	941	0	0
2	1-W	3468	0	3509	0	0
2	1-Y	3468	0	3509	0	0
2	2-W	3468	0	3509	0	0
2	2-Y	3468	0	3509	0	0
2	3-W	3468	0	3509	0	0
2	3-Y	3468	0	3509	0	0
2	4-W	3468	0	3509	0	0
2	4-Y	3468	0	3509	0	0
2	5-W	3468	0	3509	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	5-Y	3468	0	3509	0	0
2	6-W	3468	0	3509	0	0
2	6-Y	3468	0	3509	0	0
2	7-W	3468	0	3509	0	0
2	7-Y	3468	0	3509	0	0
2	8-W	3468	0	3509	0	0
2	8-Y	3468	0	3509	0	0
3	1-X	13	0	5	0	0
3	2-X	13	0	5	0	0
3	3-X	13	0	5	0	0
3	4-X	13	0	5	0	0
3	5-X	13	0	5	0	0
3	6-X	13	0	5	0	0
3	7-X	13	0	5	0	0
3	8-X	13	0	5	0	0
4	1-W	300	0	0	0	0
4	1-X	103	0	0	0	0
4	1-Y	317	0	0	0	0
4	1-Z	134	0	0	0	0
4	2-W	304	0	0	0	0
4	2-X	107	0	0	0	0
4	2-Y	309	0	0	0	0
4	2-Z	134	0	0	0	0
4	3-W	298	0	0	0	0
4	3-X	108	0	0	0	0
4	3-Y	313	0	0	0	0
4	3-Z	135	0	0	0	0
4	4-W	298	0	0	0	0
4	4-X	107	0	0	0	0
4	4-Y	316	0	0	0	0
4	4-Z	133	0	0	0	0
4	5-W	298	0	0	0	0
4	5-X	111	0	0	0	0
4	5-Y	313	0	0	0	0
4	5-Z	132	0	0	0	0
4	6-W	299	0	0	0	0
4	6-X	109	0	0	0	0
4	6-Y	319	0	0	0	0
4	6-Z	127	0	0	0	0
4	7-W	298	0	0	0	0
4	7-X	111	0	0	0	0
4	7-Y	313	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	7-Z	132	0	0	0	0
4	8-W	305	0	0	0	0
4	8-X	106	0	0	0	0
4	8-Y	312	0	0	0	0
4	8-Z	131	0	0	0	0
All	All	78360	0	71240	0	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 0.

There are no clashes within the asymmetric unit.

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%)	3	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%)	4	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%)	16	8
1	4-Z	124/129 (96%)	112 (90%)	10 (8%)	2 (2%)	7	2
1	5-X	124/129 (96%)	105 (85%)	18 (14%)	1 (1%)	16	8
1	5-Z	124/129 (96%)	115 (93%)	8 (6%)	1 (1%)	16	8
1	6-X	124/129 (96%)	110 (89%)	12 (10%)	2 (2%)	7	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7-Z	124/129 (96%)	112 (90%)	11 (9%)	1 (1%)	16	8
1	8-X	124/129 (96%)	115 (93%)	8 (6%)	1 (1%)	16	8
1	8-Z	124/129 (96%)	110 (89%)	11 (9%)	3 (2%)	4	1
2	1-W	458/461 (99%)	421 (92%)	33 (7%)	4 (1%)	14	6
2	1-Y	458/461 (99%)	419 (92%)	30 (7%)	9 (2%)	6	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%)	18	10
2	3-W	458/461 (99%)	416 (91%)	38 (8%)	4 (1%)	14	6
2	3-Y	458/461 (99%)	423 (92%)	31 (7%)	4 (1%)	14	6
2	4-W	458/461 (99%)	420 (92%)	34 (7%)	4 (1%)	14	6
2	4-Y	458/461 (99%)	431 (94%)	24 (5%)	3 (1%)	18	10
2	5-W	458/461 (99%)	427 (93%)	27 (6%)	4 (1%)	14	6
2	5-Y	458/461 (99%)	424 (93%)	31 (7%)	3 (1%)	18	10
2	6-W	458/461 (99%)	414 (90%)	37 (8%)	7 (2%)	8	2
2	6-Y	458/461 (99%)	422 (92%)	31 (7%)	5 (1%)	11	4
2	7-W	458/461 (99%)	425 (93%)	31 (7%)	2 (0%)	30	21
2	7-Y	458/461 (99%)	411 (90%)	37 (8%)	10 (2%)	5	1
2	8-W	458/461 (99%)	422 (92%)	35 (8%)	1 (0%)	43	36
2	8-Y	458/461 (99%)	428 (93%)	26 (6%)	4 (1%)	14	6
All	All	9312/9440 (99%)	8572 (92%)	654 (7%)	86 (1%)	14	6

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 ⓘ

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%)	115 (98%)	2 (2%)	53	49
1	1-Z	117/120 (98%)	114 (97%)	3 (3%)	40	33
1	2-X	117/120 (98%)	115 (98%)	2 (2%)	53	49
1	2-Z	117/120 (98%)	114 (97%)	3 (3%)	40	33
1	3-X	117/120 (98%)	115 (98%)	2 (2%)	53	49
1	3-Z	117/120 (98%)	114 (97%)	3 (3%)	40	33
1	4-X	117/120 (98%)	115 (98%)	2 (2%)	53	49
1	4-Z	117/120 (98%)	114 (97%)	3 (3%)	40	33
1	5-X	117/120 (98%)	115 (98%)	2 (2%)	53	49
1	5-Z	117/120 (98%)	114 (97%)	3 (3%)	40	33
1	6-X	117/120 (98%)	115 (98%)	2 (2%)	53	49
1	6-Z	117/120 (98%)	114 (97%)	3 (3%)	40	33
1	7-X	117/120 (98%)	115 (98%)	2 (2%)	53	49
1	7-Z	117/120 (98%)	114 (97%)	3 (3%)	40	33
1	8-X	117/120 (98%)	115 (98%)	2 (2%)	53	49
1	8-Z	117/120 (98%)	114 (97%)	3 (3%)	40	33
2	1-W	396/397 (100%)	389 (98%)	7 (2%)	51	47
2	1-Y	396/397 (100%)	390 (98%)	6 (2%)	57	54
2	2-W	396/397 (100%)	389 (98%)	7 (2%)	51	47
2	2-Y	396/397 (100%)	390 (98%)	6 (2%)	57	54
2	3-W	396/397 (100%)	389 (98%)	7 (2%)	51	47
2	3-Y	396/397 (100%)	390 (98%)	6 (2%)	57	54
2	4-W	396/397 (100%)	389 (98%)	7 (2%)	51	47
2	4-Y	396/397 (100%)	390 (98%)	6 (2%)	57	54
2	5-W	396/397 (100%)	389 (98%)	7 (2%)	51	47
2	5-Y	396/397 (100%)	390 (98%)	6 (2%)	57	54
2	6-W	396/397 (100%)	389 (98%)	7 (2%)	51	47
2	6-Y	396/397 (100%)	390 (98%)	6 (2%)	57	54
2	7-W	396/397 (100%)	389 (98%)	7 (2%)	51	47
2	7-Y	396/397 (100%)	390 (98%)	6 (2%)	57	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	8-W	396/397 (100%)	389 (98%)	7 (2%)	51	47
2	8-Y	396/397 (100%)	390 (98%)	6 (2%)	57	54
All	All	8208/8272 (99%)	8064 (98%)	144 (2%)	51	47

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	7-W	262	ILE
2	8-Y	429	GLU
1	7-Z	100	SER
2	8-W	216	ARG
2	3-Y	96	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 185 such sidechains are listed below:

Mol	Chain	Res	Type
2	5-Y	397	HIS
2	6-Y	430	GLN
2	6-W	73	HIS
1	6-Z	76	ASN
2	7-W	346	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 oligosaccharides 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	4-X	900	-	12,12,12	4.35	7 (58%)	17,17,17	5.56	10 (58%)
3	CIT	8-X	900	-	12,12,12	4.20	7 (58%)	17,17,17	5.62	11 (64%)
3	CIT	2-X	900	-	12,12,12	4.56	6 (50%)	17,17,17	5.53	10 (58%)
3	CIT	1-X	900	-	12,12,12	4.58	6 (50%)	17,17,17	5.88	11 (64%)
3	CIT	3-X	900	-	12,12,12	4.35	6 (50%)	17,17,17	5.59	11 (64%)
3	CIT	6-X	900	-	12,12,12	4.70	7 (58%)	17,17,17	5.47	10 (58%)
3	CIT	7-X	900	-	12,12,12	4.49	6 (50%)	17,17,17	5.55	10 (58%)
3	CIT	5-X	900	-	12,12,12	4.89	6 (50%)	17,17,17	5.55	11 (64%)

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	4-X	900	-	-	8/16/16/16	-
3	CIT	8-X	900	-	-	5/16/16/16	-
3	CIT	2-X	900	-	-	5/16/16/16	-
3	CIT	1-X	900	-	-	4/16/16/16	-
3	CIT	3-X	900	-	-	7/16/16/16	-
3	CIT	6-X	900	-	-	5/16/16/16	-
3	CIT	7-X	900	-	-	6/16/16/16	-
3	CIT	5-X	900	-	-	3/16/16/16	-

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	5-X	900	CIT	C3-C6	15.00	1.69	1.53
3	6-X	900	CIT	C3-C6	14.32	1.68	1.53
3	1-X	900	CIT	C3-C6	13.98	1.68	1.53
3	2-X	900	CIT	C3-C6	13.81	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	7-X	900	CIT	C3-C6	13.58	1.67	1.53

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-X	900	CIT	O7-C3-C6	-14.19	88.84	108.96
3	4-X	900	CIT	O7-C3-C6	-13.97	89.14	108.96
3	7-X	900	CIT	O7-C3-C6	-13.96	89.16	108.96
3	2-X	900	CIT	O7-C3-C6	-13.86	89.30	108.96
3	3-X	900	CIT	O7-C3-C6	-13.80	89.39	108.96

There are no chirality outliers.

5 of 43 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.

No monomer is involved in short contacts.

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	1-X	126/129 (97%)	1.83	43 (34%) ⓘ ⓘ	2, 3, 4, 5	126 (100%)
1	1-Z	126/129 (97%)	1.78	37 (29%) ⓘ ⓘ	2, 2, 4, 5	126 (100%)
1	2-X	0/129	-	-	-	-
1	2-Z	0/129	-	-	-	-
1	3-X	0/129	-	-	-	-
1	3-Z	0/129	-	-	-	-
1	4-X	0/129	-	-	-	-
1	4-Z	0/129	-	-	-	-
1	5-X	0/129	-	-	-	-
1	5-Z	0/129	-	-	-	-
1	6-X	0/129	-	-	-	-
1	6-Z	0/129	-	-	-	-
1	7-X	0/129	-	-	-	-
1	7-Z	0/129	-	-	-	-
1	8-X	0/129	-	-	-	-
1	8-Z	0/129	-	-	-	-
2	1-W	460/461 (99%)	1.60	120 (26%) ⓘ ⓘ	1, 3, 4, 5	460 (100%)
2	1-Y	460/461 (99%)	1.80	163 (35%) ⓘ ⓘ	1, 3, 4, 5	460 (100%)
2	2-W	0/461	-	-	-	-
2	2-Y	0/461	-	-	-	-
2	3-W	0/461	-	-	-	-
2	3-Y	0/461	-	-	-	-
2	4-W	0/461	-	-	-	-
2	4-Y	0/461	-	-	-	-
2	5-W	0/461	-	-	-	-
2	5-Y	0/461	-	-	-	-
2	6-W	0/461	-	-	-	-
2	6-Y	0/461	-	-	-	-
2	7-W	0/461	-	-	-	-
2	7-Y	0/461	-	-	-	-
2	8-W	0/461	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	8-Y	0/461	-	-	-	-
All	All	1172/9440 (12%)	1.72	363 (30%) 1 1	1, 3, 4, 5	1172 (100%)

The worst 5 of 363 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-Z	89	GLY	10.4
1	1-X	70	GLY	8.8
2	1-Y	42	ALA	8.3
2	1-Y	55	PRO	7.9
2	1-Y	310	PRO	6.9

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
3	CIT	1-X	900	13/13	0.48	0.20	12,22,25,27	13
3	CIT	2-X	900	13/13	-	-	19,24,28,28	13
3	CIT	3-X	900	13/13	-	-	21,24,29,31	13
3	CIT	4-X	900	13/13	-	-	18,26,29,30	13
3	CIT	5-X	900	13/13	-	-	10,18,22,26	13
3	CIT	6-X	900	13/13	-	-	18,24,26,27	13
3	CIT	7-X	900	13/13	-	-	20,24,28,29	13
3	CIT	8-X	900	13/13	-	-	1,25,30,32	13

6.5 Other polymers [i](#)

There are no such residues in this entry.