



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 11:29 PM UTC

PDB ID : 9IAM / pdb\_00009iam  
Title : Structure of cyclodi peptide synthase from *Nocardia brasiliensis* (Nbra-CDPS) in complex with alanylated RNA microhelices analogues mimicking Ala-tRNA-Ala substrate  
Authors : Marouf, Z.; Charbonnier, J.B.; Fernandez Varela, P.; Legrand, P.  
Deposited on : 2025-02-11  
Resolution : 3.61 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	4-5-2 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

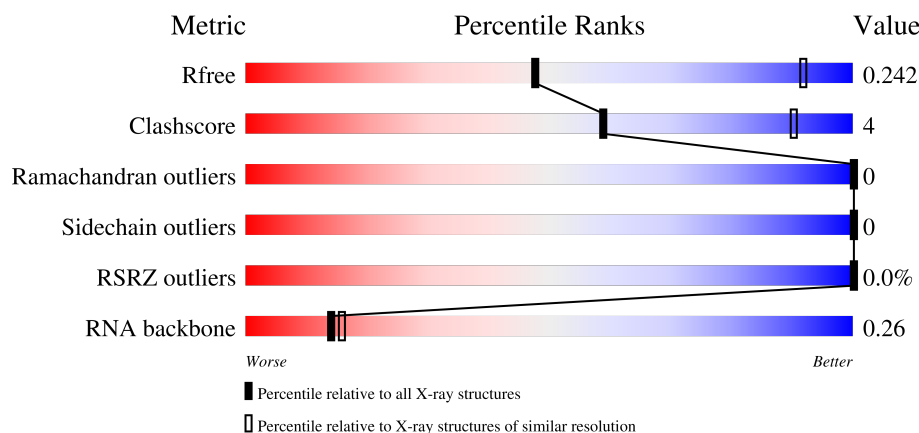
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 3.61 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	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)
RNA backbone	3983	1018 (4.18-3.06)

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	248	 82% 9% 8%
1	B	248	 85% 7% 8%
1	C	248	 80% 12% 8%
1	D	248	 80% 12% 8%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	E	248	
1	F	248	
1	G	248	
1	H	248	
1	I	248	
1	J	248	
1	K	248	
1	L	248	
1	M	248	
1	N	248	
2	O	22	
2	P	22	
2	Q	22	
2	R	22	
2	T	22	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 54091 atoms, of which 26218 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 Cyclodipeptide synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	227	Total	C	H	N	O	S	0	0	0
			3616	1144	1789	338	340	5			
1	B	228	Total	C	H	N	O	S	0	0	0
			3627	1147	1794	339	342	5			
1	C	227	Total	C	H	N	O	S	0	0	0
			3613	1143	1787	338	340	5			
1	D	228	Total	C	H	N	O	S	0	0	0
			3627	1147	1794	339	342	5			
1	E	227	Total	C	H	N	O	S	0	0	0
			3613	1143	1787	338	340	5			
1	F	227	Total	C	H	N	O	S	0	0	0
			3613	1143	1787	338	340	5			
1	G	227	Total	C	H	N	O	S	0	0	0
			3613	1143	1787	338	340	5			
1	H	228	Total	C	H	N	O	S	0	0	0
			3627	1147	1794	339	342	5			
1	I	227	Total	C	H	N	O	S	0	0	0
			3613	1143	1787	338	340	5			
1	J	227	Total	C	H	N	O	S	0	0	0
			3613	1143	1787	338	340	5			
1	K	227	Total	C	H	N	O	S	0	0	0
			3613	1143	1787	338	340	5			
1	L	227	Total	C	H	N	O	S	0	0	0
			3616	1144	1789	338	340	5			
1	M	227	Total	C	H	N	O	S	0	0	0
			3613	1143	1787	338	340	5			
1	N	228	Total	C	H	N	O	S	0	0	0
			3627	1147	1794	339	342	5			

There are 154 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP K0F6G5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP K0F6G5
A	34	ALA	SER	conflict	UNP K0F6G5
A	240	ARG	-	expression tag	UNP K0F6G5
A	241	SER	-	expression tag	UNP K0F6G5
A	242	HIS	-	expression tag	UNP K0F6G5
A	243	HIS	-	expression tag	UNP K0F6G5
A	244	HIS	-	expression tag	UNP K0F6G5
A	245	HIS	-	expression tag	UNP K0F6G5
A	246	HIS	-	expression tag	UNP K0F6G5
A	247	HIS	-	expression tag	UNP K0F6G5
B	0	MET	-	initiating methionine	UNP K0F6G5
B	1	ALA	-	expression tag	UNP K0F6G5
B	34	ALA	SER	conflict	UNP K0F6G5
B	240	ARG	-	expression tag	UNP K0F6G5
B	241	SER	-	expression tag	UNP K0F6G5
B	242	HIS	-	expression tag	UNP K0F6G5
B	243	HIS	-	expression tag	UNP K0F6G5
B	244	HIS	-	expression tag	UNP K0F6G5
B	245	HIS	-	expression tag	UNP K0F6G5
B	246	HIS	-	expression tag	UNP K0F6G5
B	247	HIS	-	expression tag	UNP K0F6G5
C	0	MET	-	initiating methionine	UNP K0F6G5
C	1	ALA	-	expression tag	UNP K0F6G5
C	34	ALA	SER	conflict	UNP K0F6G5
C	240	ARG	-	expression tag	UNP K0F6G5
C	241	SER	-	expression tag	UNP K0F6G5
C	242	HIS	-	expression tag	UNP K0F6G5
C	243	HIS	-	expression tag	UNP K0F6G5
C	244	HIS	-	expression tag	UNP K0F6G5
C	245	HIS	-	expression tag	UNP K0F6G5
C	246	HIS	-	expression tag	UNP K0F6G5
C	247	HIS	-	expression tag	UNP K0F6G5
D	0	MET	-	initiating methionine	UNP K0F6G5
D	1	ALA	-	expression tag	UNP K0F6G5
D	34	ALA	SER	conflict	UNP K0F6G5
D	240	ARG	-	expression tag	UNP K0F6G5
D	241	SER	-	expression tag	UNP K0F6G5
D	242	HIS	-	expression tag	UNP K0F6G5
D	243	HIS	-	expression tag	UNP K0F6G5
D	244	HIS	-	expression tag	UNP K0F6G5
D	245	HIS	-	expression tag	UNP K0F6G5
D	246	HIS	-	expression tag	UNP K0F6G5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	247	HIS	-	expression tag	UNP K0F6G5
E	0	MET	-	initiating methionine	UNP K0F6G5
E	1	ALA	-	expression tag	UNP K0F6G5
E	34	ALA	SER	conflict	UNP K0F6G5
E	240	ARG	-	expression tag	UNP K0F6G5
E	241	SER	-	expression tag	UNP K0F6G5
E	242	HIS	-	expression tag	UNP K0F6G5
E	243	HIS	-	expression tag	UNP K0F6G5
E	244	HIS	-	expression tag	UNP K0F6G5
E	245	HIS	-	expression tag	UNP K0F6G5
E	246	HIS	-	expression tag	UNP K0F6G5
E	247	HIS	-	expression tag	UNP K0F6G5
F	0	MET	-	initiating methionine	UNP K0F6G5
F	1	ALA	-	expression tag	UNP K0F6G5
F	34	ALA	SER	conflict	UNP K0F6G5
F	240	ARG	-	expression tag	UNP K0F6G5
F	241	SER	-	expression tag	UNP K0F6G5
F	242	HIS	-	expression tag	UNP K0F6G5
F	243	HIS	-	expression tag	UNP K0F6G5
F	244	HIS	-	expression tag	UNP K0F6G5
F	245	HIS	-	expression tag	UNP K0F6G5
F	246	HIS	-	expression tag	UNP K0F6G5
F	247	HIS	-	expression tag	UNP K0F6G5
G	0	MET	-	initiating methionine	UNP K0F6G5
G	1	ALA	-	expression tag	UNP K0F6G5
G	34	ALA	SER	conflict	UNP K0F6G5
G	240	ARG	-	expression tag	UNP K0F6G5
G	241	SER	-	expression tag	UNP K0F6G5
G	242	HIS	-	expression tag	UNP K0F6G5
G	243	HIS	-	expression tag	UNP K0F6G5
G	244	HIS	-	expression tag	UNP K0F6G5
G	245	HIS	-	expression tag	UNP K0F6G5
G	246	HIS	-	expression tag	UNP K0F6G5
G	247	HIS	-	expression tag	UNP K0F6G5
H	0	MET	-	initiating methionine	UNP K0F6G5
H	1	ALA	-	expression tag	UNP K0F6G5
H	34	ALA	SER	conflict	UNP K0F6G5
H	240	ARG	-	expression tag	UNP K0F6G5
H	241	SER	-	expression tag	UNP K0F6G5
H	242	HIS	-	expression tag	UNP K0F6G5
H	243	HIS	-	expression tag	UNP K0F6G5
H	244	HIS	-	expression tag	UNP K0F6G5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
H	245	HIS	-	expression tag	UNP K0F6G5
H	246	HIS	-	expression tag	UNP K0F6G5
H	247	HIS	-	expression tag	UNP K0F6G5
I	0	MET	-	initiating methionine	UNP K0F6G5
I	1	ALA	-	expression tag	UNP K0F6G5
I	34	ALA	SER	conflict	UNP K0F6G5
I	240	ARG	-	expression tag	UNP K0F6G5
I	241	SER	-	expression tag	UNP K0F6G5
I	242	HIS	-	expression tag	UNP K0F6G5
I	243	HIS	-	expression tag	UNP K0F6G5
I	244	HIS	-	expression tag	UNP K0F6G5
I	245	HIS	-	expression tag	UNP K0F6G5
I	246	HIS	-	expression tag	UNP K0F6G5
I	247	HIS	-	expression tag	UNP K0F6G5
J	0	MET	-	initiating methionine	UNP K0F6G5
J	1	ALA	-	expression tag	UNP K0F6G5
J	34	ALA	SER	conflict	UNP K0F6G5
J	240	ARG	-	expression tag	UNP K0F6G5
J	241	SER	-	expression tag	UNP K0F6G5
J	242	HIS	-	expression tag	UNP K0F6G5
J	243	HIS	-	expression tag	UNP K0F6G5
J	244	HIS	-	expression tag	UNP K0F6G5
J	245	HIS	-	expression tag	UNP K0F6G5
J	246	HIS	-	expression tag	UNP K0F6G5
J	247	HIS	-	expression tag	UNP K0F6G5
K	0	MET	-	initiating methionine	UNP K0F6G5
K	1	ALA	-	expression tag	UNP K0F6G5
K	34	ALA	SER	conflict	UNP K0F6G5
K	240	ARG	-	expression tag	UNP K0F6G5
K	241	SER	-	expression tag	UNP K0F6G5
K	242	HIS	-	expression tag	UNP K0F6G5
K	243	HIS	-	expression tag	UNP K0F6G5
K	244	HIS	-	expression tag	UNP K0F6G5
K	245	HIS	-	expression tag	UNP K0F6G5
K	246	HIS	-	expression tag	UNP K0F6G5
K	247	HIS	-	expression tag	UNP K0F6G5
L	0	MET	-	initiating methionine	UNP K0F6G5
L	1	ALA	-	expression tag	UNP K0F6G5
L	34	ALA	SER	conflict	UNP K0F6G5
L	240	ARG	-	expression tag	UNP K0F6G5
L	241	SER	-	expression tag	UNP K0F6G5
L	242	HIS	-	expression tag	UNP K0F6G5

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	243	HIS	-	expression tag	UNP K0F6G5
L	244	HIS	-	expression tag	UNP K0F6G5
L	245	HIS	-	expression tag	UNP K0F6G5
L	246	HIS	-	expression tag	UNP K0F6G5
L	247	HIS	-	expression tag	UNP K0F6G5
M	0	MET	-	initiating methionine	UNP K0F6G5
M	1	ALA	-	expression tag	UNP K0F6G5
M	34	ALA	SER	conflict	UNP K0F6G5
M	240	ARG	-	expression tag	UNP K0F6G5
M	241	SER	-	expression tag	UNP K0F6G5
M	242	HIS	-	expression tag	UNP K0F6G5
M	243	HIS	-	expression tag	UNP K0F6G5
M	244	HIS	-	expression tag	UNP K0F6G5
M	245	HIS	-	expression tag	UNP K0F6G5
M	246	HIS	-	expression tag	UNP K0F6G5
M	247	HIS	-	expression tag	UNP K0F6G5
N	0	MET	-	initiating methionine	UNP K0F6G5
N	1	ALA	-	expression tag	UNP K0F6G5
N	34	ALA	SER	conflict	UNP K0F6G5
N	240	ARG	-	expression tag	UNP K0F6G5
N	241	SER	-	expression tag	UNP K0F6G5
N	242	HIS	-	expression tag	UNP K0F6G5
N	243	HIS	-	expression tag	UNP K0F6G5
N	244	HIS	-	expression tag	UNP K0F6G5
N	245	HIS	-	expression tag	UNP K0F6G5
N	246	HIS	-	expression tag	UNP K0F6G5
N	247	HIS	-	expression tag	UNP K0F6G5

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


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	O	22	Total	C	H	N	O	P	0	0	0
			717	211	245	83	156	22			
2	P	22	Total	C	H	N	O	P	0	0	0
			717	211	245	83	156	22			
2	R	21	Total	C	H	N	O	P	2	0	0
			671	198	226	76	150	21			
2	Q	21	Total	C	H	N	O	P	0	0	0
			671	198	226	76	150	21			
2	T	21	Total	C	H	N	O	P	0	0	0
			671	198	226	76	150	21			



### 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.

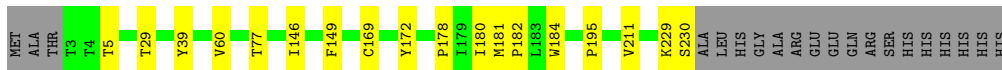
- Molecule 1: Cyclodipeptide synthase

Chain A: 




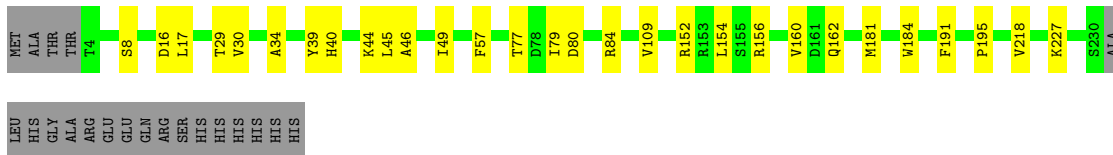
- Molecule 1: Cyclodipeptide synthase

Chain B: 




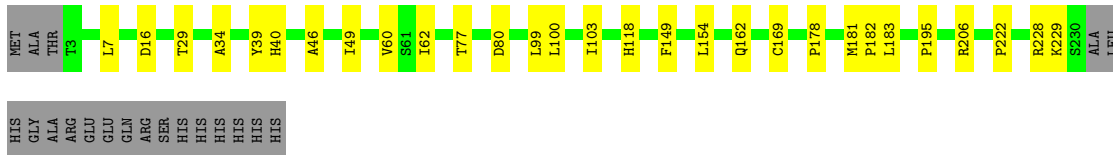
- Molecule 1: Cyclodipeptide synthase

Chain C: 




- Molecule 1: Cyclodipeptide synthase

Chain D: 

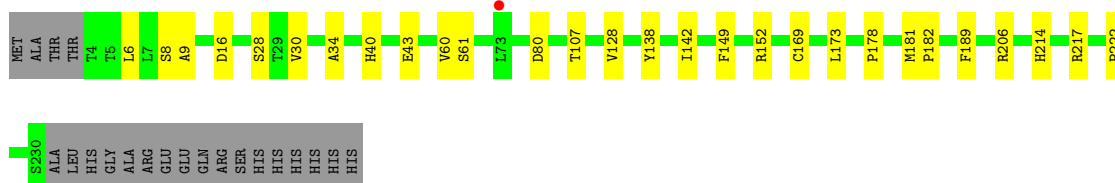


- Molecule 1: Cyclodipeptide synthase

Chain E: 

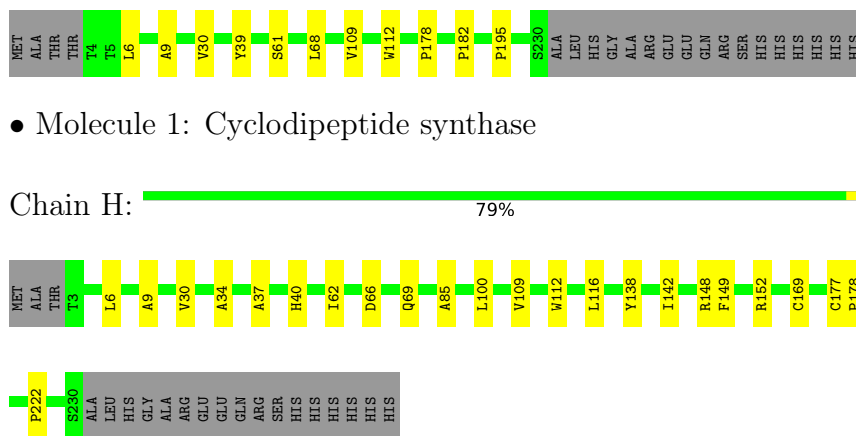
- Molecule 1: Cyclodipeptide synthase

Chain F:  80% 11% 8%

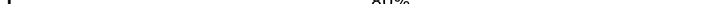


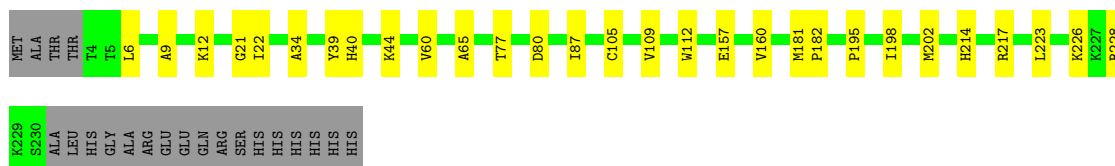
- Molecule 1: Cyclodipeptide synthase

Chain G:  87% . 8%



- Molecule 1: Cyclodipeptide synthase

Chain I:  80% 12% 8%




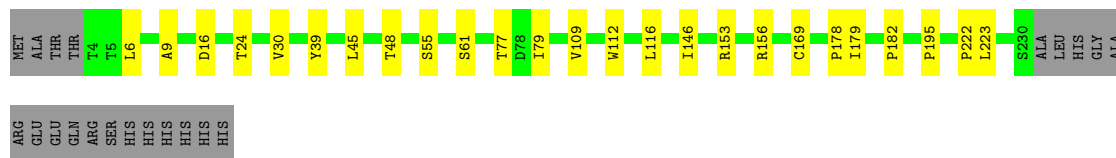
- Molecule 1: Cyclodipeptide synthase

Chain J:  85% 6% 8%




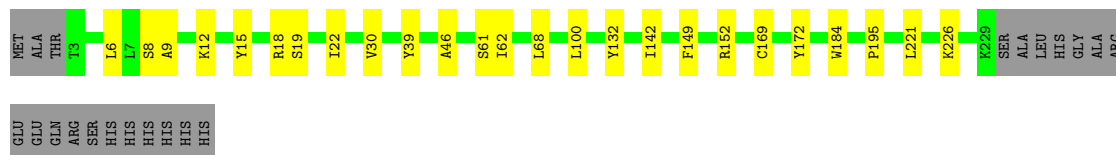
- Molecule 1: Cyclodipeptide synthase

Chain K:  81% 10% 8%




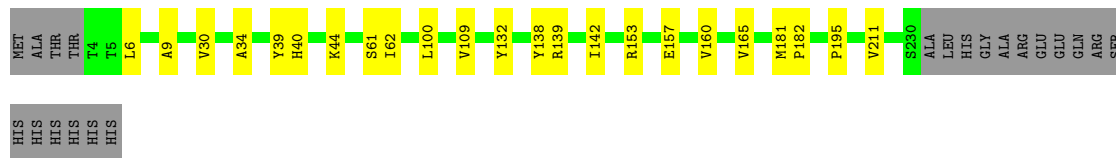
- Molecule 1: Cyclodipeptide synthase

Chain L:  81% 10% 8%




- Molecule 1: Cyclodipeptide synthase

Chain M:  82% 9% 8%



- Molecule 1: Cyclodipeptide synthase

Chain N:  87% 5% 8%



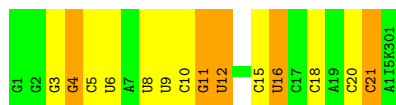
- Molecule 2: RNA (5'-R(P\*GP\*GP\*GP\*GP\*CP\*UP\*AP\*UP\*UP\*CP\*GP\*UP\*AP\*GP\*CP\*UP\*CP\*CP\*AP\*CP\*C)-3')

Chain O:  50% 32% 18%



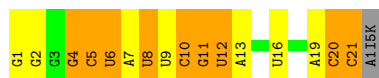
- Molecule 2: RNA (5'-R(P\*GP\*GP\*GP\*GP\*CP\*UP\*AP\*UP\*UP\*CP\*GP\*UP\*AP\*GP\*CP\*UP\*CP\*CP\*AP\*CP\*C)-3')

Chain P:  36% 41% 23%



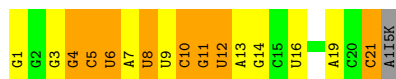
● Molecule 2: RNA (5'-R(P\*GP\*GP\*GP\*GP\*CP\*UP\*AP\*UP\*UP\*CP\*GP\*UP\*AP\*GP\*CP\*UP\*CP\*CP\*AP\*CP\*C)-3')

Chain R: 23% 32% 41% 5%



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

Chain Q: 23% 36% 36% 5%



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

Chain T: 36% 32% 27% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.00Å 170.13Å 319.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.30 – 3.61 49.30 – 3.61	Depositor EDS
% Data completeness (in resolution range)	65.5 (49.30-3.61) 65.4 (49.30-3.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.192 , 0.244 0.194 , 0.242	Depositor DCC
$R_{free}$ test set	2000 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	54091	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: A1I5K

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	0.24	0/1868	0.47	0/2536
1	B	0.28	1/1874 (0.1%)	0.48	0/2544
1	C	0.26	0/1867	0.46	0/2534
1	D	0.22	0/1874	0.46	0/2544
1	E	0.24	0/1867	0.48	0/2534
1	F	0.22	0/1867	0.43	0/2534
1	G	0.25	0/1867	0.44	0/2534
1	H	0.21	0/1874	0.43	0/2544
1	I	0.23	0/1867	0.46	0/2534
1	J	0.21	0/1867	0.43	0/2534
1	K	0.23	0/1867	0.43	0/2534
1	L	0.22	0/1868	0.46	0/2536
1	M	0.27	1/1867 (0.1%)	0.44	0/2534
1	N	0.21	0/1874	0.43	0/2544
2	O	0.30	0/495	0.60	0/767
2	P	0.30	0/495	0.62	0/767
2	Q	0.24	0/495	0.58	0/767
2	R	0.24	0/495	0.65	0/767
2	T	0.22	0/495	0.55	0/767
All	All	0.24	2/28643 (0.0%)	0.47	0/39355

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	211	VAL	CA-CB	-6.37	1.50	1.54
1	M	211	VAL	CA-CB	-5.07	1.51	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1827	1789	1789	19	0
1	B	1833	1794	1794	12	0
1	C	1826	1787	1787	22	0
1	D	1833	1794	1794	19	0
1	E	1826	1787	1787	15	0
1	F	1826	1787	1787	18	0
1	G	1826	1787	1787	6	0
1	H	1833	1794	1794	17	0
1	I	1826	1787	1787	19	0
1	J	1826	1787	1787	8	0
1	K	1826	1787	1787	14	0
1	L	1827	1789	1789	18	0
1	M	1826	1787	1787	12	0
1	N	1833	1794	1794	7	0
2	O	472	245	226	4	0
2	P	472	245	226	9	0
2	Q	445	226	227	10	0
2	R	445	226	227	15	0
2	T	445	226	227	9	0
All	All	27873	26218	26183	238	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 4.

All (238) 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:C:29:THR:HG22	1:C:191:PHE:HB2	1.54	0.88
1:A:77:THR:HG21	1:D:99:LEU:HD11	1.60	0.83
1:A:39:TYR:OH	2:P:20:C:O2	2.02	0.77
1:D:118:HIS:CD2	1:D:183:LEU:HD11	2.19	0.76
1:D:77:THR:HG23	1:D:80:ASP:H	1.51	0.75
1:A:79:ILE:HD11	1:D:7:LEU:O	1.94	0.68
1:L:6:LEU:HD23	1:L:9:ALA:HA	1.79	0.65
1:D:16:ASP:HB3	1:D:222:PRO:HB2	1.80	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:118:HIS:CD2	1:J:183:LEU:HD11	2.32	0.63
1:J:30:VAL:HG22	1:J:61:SER:HB3	1.79	0.62
1:E:138:TYR:CZ	1:E:142:ILE:HD11	2.34	0.62
1:G:6:LEU:HD23	1:G:9:ALA:HA	1.82	0.61
1:L:18:ARG:NE	1:L:18:ARG:HA	2.16	0.59
1:A:181:MET:HE3	1:A:202:MET:HG3	1.84	0.59
1:D:118:HIS:HD2	1:D:183:LEU:HD11	1.67	0.58
1:M:30:VAL:HG22	1:M:61:SER:HB3	1.85	0.58
1:I:21:GLY:C	1:I:22:ILE:HD12	2.29	0.58
1:J:6:LEU:HD21	1:J:228:ARG:NH2	2.19	0.58
1:E:6:LEU:HD23	1:E:9:ALA:HA	1.85	0.58
1:F:6:LEU:HD23	1:F:9:ALA:HA	1.86	0.58
1:K:6:LEU:HD23	1:K:9:ALA:HA	1.84	0.58
1:C:152:ARG:NE	2:R:21:C:O2'	2.38	0.57
2:R:4:G:O2'	2:R:5:C:OP2	2.18	0.57
1:F:152:ARG:HD3	2:T:21:C:H5''	1.88	0.56
2:P:20:C:H2'	2:P:21:C:H5''	1.88	0.56
1:C:30:VAL:HG11	1:C:184:TRP:CZ3	2.40	0.56
1:H:66:ASP:O	1:H:85:ALA:HB1	2.06	0.56
1:I:39:TYR:CD1	1:I:195:PRO:HG2	2.39	0.55
1:H:30:VAL:HG11	1:H:184:TRP:CZ3	2.42	0.55
1:H:109:VAL:HG23	1:H:109:VAL:O	2.07	0.55
1:L:18:ARG:HA	1:L:18:ARG:CZ	2.37	0.55
1:K:39:TYR:CD1	1:K:195:PRO:HG2	2.42	0.54
1:C:77:THR:HG23	1:C:80:ASP:H	1.72	0.54
1:D:228:ARG:O	1:D:229:LYS:HD2	2.08	0.54
1:C:154:LEU:HD21	1:C:162:GLN:OE1	2.08	0.53
1:C:29:THR:HG21	1:C:57:PHE:CE1	2.43	0.53
1:B:149:PHE:CD2	1:B:169:CYS:SG	3.02	0.53
1:C:109:VAL:HG23	1:C:109:VAL:O	2.08	0.53
1:F:128:VAL:HG13	1:F:138:TYR:OH	2.09	0.53
1:F:8:SER:OG	1:F:43:GLU:HG3	2.08	0.53
2:Q:11:G:H2'	2:Q:12:U:O4'	2.07	0.53
1:K:30:VAL:HG22	1:K:61:SER:HB3	1.91	0.53
1:C:30:VAL:HG11	1:C:184:TRP:CH2	2.44	0.53
1:H:6:LEU:HD23	1:H:9:ALA:HA	1.91	0.53
1:A:154:LEU:HD21	1:A:162:GLN:HE21	1.74	0.52
2:R:6:U:O2'	2:R:7:A:H5'	2.10	0.52
1:C:79:ILE:H	1:C:79:ILE:HD12	1.75	0.52
2:R:12:U:H2'	2:R:13:A:C8	2.44	0.52
2:T:6:U:O2'	2:T:7:A:H5'	2.09	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:TYR:CZ	1:F:142:ILE:HD11	2.44	0.52
1:M:39:TYR:CD1	1:M:195:PRO:HG2	2.45	0.52
1:K:16:ASP:HB3	1:K:222:PRO:HB2	1.92	0.51
2:T:13:A:C6	2:T:14:G:C6	2.98	0.51
1:I:77:THR:HG23	1:I:80:ASP:H	1.75	0.51
1:C:227:LYS:HE2	2:R:2:G:OP2	2.11	0.51
1:I:109:VAL:O	1:I:109:VAL:HG23	2.10	0.51
2:R:11:G:O2'	2:R:12:U:O4'	2.28	0.51
1:D:34:ALA:H	1:D:40:HIS:CE1	2.29	0.50
1:E:109:VAL:O	1:E:109:VAL:HG13	2.11	0.50
1:N:39:TYR:CD1	1:N:195:PRO:HG2	2.47	0.50
1:C:152:ARG:O	1:C:156:ARG:HG3	2.12	0.50
1:C:39:TYR:CD1	1:C:195:PRO:HG2	2.47	0.50
1:F:152:ARG:NE	2:T:21:C:H2'	2.27	0.50
1:B:180:ILE:HA	1:B:184:TRP:CE3	2.47	0.49
2:R:11:G:O2'	2:R:12:U:C1'	2.60	0.49
1:K:109:VAL:HG23	1:K:109:VAL:O	2.10	0.49
1:C:34:ALA:H	1:C:40:HIS:CE1	2.31	0.49
1:N:19:SER:HA	1:N:22:ILE:HG12	1.95	0.49
1:A:39:TYR:OH	2:P:20:C:C2	2.60	0.49
1:D:39:TYR:CD1	1:D:195:PRO:HG2	2.47	0.49
1:N:195:PRO:HA	1:N:223:LEU:HB2	1.95	0.49
1:C:154:LEU:HD23	1:C:160:VAL:HG22	1.94	0.48
1:F:30:VAL:HG22	1:F:61:SER:HB3	1.95	0.48
1:G:109:VAL:O	1:G:109:VAL:HG23	2.12	0.48
1:M:62:ILE:HD13	1:M:100:LEU:HD22	1.94	0.48
1:N:149:PHE:CD2	1:N:169:CYS:SG	3.06	0.48
1:A:37:ALA:HB3	1:A:40:HIS:ND1	2.28	0.48
2:T:5:C:O2'	2:T:6:U:OP2	2.30	0.48
1:A:181:MET:HB3	1:A:182:PRO:HD3	1.95	0.48
2:R:8:U:C4	2:R:10:C:N3	2.82	0.48
1:J:67:THR:HG21	1:J:113:ASP:OD2	2.13	0.48
2:R:20:C:O5'	2:R:20:C:H6	1.97	0.48
1:B:39:TYR:CD1	1:B:195:PRO:HG2	2.49	0.48
1:A:198:ILE:HB	1:A:220:TRP:CD1	2.48	0.48
1:D:16:ASP:CB	1:D:222:PRO:HB2	2.43	0.48
1:M:157:GLU:CD	1:M:160:VAL:HG11	2.39	0.48
1:E:60:VAL:HG23	1:E:105:CYS:SG	2.55	0.47
1:E:157:GLU:CD	1:E:160:VAL:HG13	2.38	0.47
1:F:169:CYS:O	1:F:173:LEU:HD13	2.15	0.47
2:P:11:G:O2'	2:P:12:U:O4'	2.22	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:8:U:O2'	2:R:11:G:N7	2.48	0.47
1:D:149:PHE:CD2	1:D:169:CYS:SG	3.08	0.47
1:D:154:LEU:HD21	1:D:162:GLN:HE21	1.79	0.47
1:L:19:SER:HA	1:L:22:ILE:HG12	1.97	0.47
1:C:77:THR:OG1	1:C:79:ILE:HD12	2.15	0.47
1:K:195:PRO:HA	1:K:223:LEU:HB2	1.97	0.47
2:T:12:U:H2'	2:T:13:A:C8	2.49	0.47
1:H:177:CYS:O	1:H:182:PRO:HD2	2.15	0.46
1:H:112:TRP:CD1	1:H:116:LEU:HD11	2.50	0.46
1:I:12:LYS:HD3	1:I:226:LYS:HE2	1.97	0.46
1:N:178:PRO:O	1:N:182:PRO:HG2	2.15	0.46
1:H:37:ALA:HB3	1:H:40:HIS:ND1	2.29	0.46
2:Q:5:C:O2'	2:Q:6:U:OP2	2.29	0.46
1:I:34:ALA:H	1:I:40:HIS:CE1	2.34	0.46
1:D:62:ILE:HD13	1:D:100:LEU:HD22	1.96	0.46
1:L:39:TYR:CD1	1:L:195:PRO:HG2	2.50	0.46
1:L:152:ARG:HD3	2:Q:21:C:H5'	1.96	0.46
1:I:6:LEU:HD21	1:I:228:ARG:NH2	2.30	0.46
1:K:153:ARG:HE	1:K:156:ARG:HH21	1.64	0.46
1:A:109:VAL:HG23	1:A:109:VAL:O	2.16	0.46
1:G:39:TYR:CD1	1:G:195:PRO:HG2	2.51	0.46
1:A:172:TYR:CD1	1:A:172:TYR:C	2.93	0.46
1:F:152:ARG:HD3	2:T:21:C:C5'	2.46	0.46
1:H:181:MET:HA	1:H:218:VAL:HG11	1.98	0.46
1:L:62:ILE:HD13	1:L:100:LEU:HD22	1.98	0.46
1:F:60:VAL:O	1:F:107:THR:HA	2.16	0.45
1:H:148:ARG:HH12	1:H:200:ALA:HB3	1.81	0.45
1:B:178:PRO:O	1:B:182:PRO:HG2	2.16	0.45
1:F:149:PHE:HD1	1:F:152:ARG:NH1	2.15	0.45
1:G:178:PRO:O	1:G:182:PRO:HG2	2.16	0.45
1:H:149:PHE:HD1	1:H:152:ARG:NH1	2.14	0.45
2:Q:3:G:C2'	2:Q:4:G:H5'	2.46	0.45
1:D:181:MET:SD	1:D:206:ARG:HB2	2.56	0.45
1:A:6:LEU:HD23	1:A:228:ARG:HH12	1.80	0.45
1:A:79:ILE:HD11	1:D:7:LEU:C	2.41	0.45
1:M:153:ARG:NH1	1:M:165:VAL:HG22	2.31	0.45
1:H:138:TYR:CZ	1:H:142:ILE:HD11	2.51	0.45
1:H:214:HIS:CG	1:H:217:ARG:NH1	2.84	0.45
1:C:80:ASP:OD2	1:C:84:ARG:NH1	2.50	0.45
1:M:39:TYR:HA	1:M:44:LYS:HD2	1.99	0.45
1:H:62:ILE:HD13	1:H:100:LEU:HD22	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:PHE:CD2	1:H:169:CYS:SG	3.10	0.45
1:J:34:ALA:H	1:J:40:HIS:CE1	2.34	0.45
1:J:147:ASP:O	1:J:151:GLU:HG2	2.17	0.45
2:P:15:C:H2'	2:P:16:U:O4'	2.17	0.45
2:Q:4:G:O2'	2:Q:5:C:OP2	2.26	0.44
1:E:18:ARG:C	1:E:20:ASP:H	2.25	0.44
1:L:12:LYS:HD3	1:L:226:LYS:HE2	2.00	0.44
1:D:178:PRO:O	1:D:182:PRO:HG2	2.17	0.44
1:A:6:LEU:CD2	1:A:228:ARG:HH12	2.30	0.44
1:A:6:LEU:HD13	1:F:80:ASP:HB2	2.00	0.44
1:B:229:LYS:O	1:B:230:SER:C	2.60	0.44
1:A:144:SER:O	1:A:148:ARG:HG3	2.16	0.44
1:N:128:VAL:HG22	1:N:209:PHE:CE2	2.52	0.44
2:Q:12:U:H2'	2:Q:13:A:C8	2.52	0.44
1:L:15:TYR:CE1	1:L:221:LEU:HD13	2.53	0.44
2:Q:1:G:N2	2:Q:19:A:H1'	2.33	0.43
2:Q:14:G:O5'	2:Q:14:G:H8	2.01	0.43
1:N:130:HIS:CE1	1:N:134:THR:HG21	2.53	0.43
2:R:21:C:O2	2:R:21:C:O4'	2.34	0.43
1:K:112:TRP:CZ2	1:K:179:ILE:HD12	2.53	0.43
1:L:172:TYR:CD1	1:L:172:TYR:C	2.95	0.43
1:M:109:VAL:HG23	1:M:109:VAL:O	2.18	0.43
1:B:29:THR:CG2	1:B:60:VAL:HG22	2.49	0.43
1:J:39:TYR:HA	1:J:44:LYS:HD2	2.00	0.43
1:K:24:THR:CB	1:K:55:SER:HB3	2.48	0.43
1:H:197:ARG:HG2	1:H:222:PRO:CG	2.49	0.43
1:I:60:VAL:HG23	1:I:105:CYS:SG	2.58	0.43
2:T:7:A:C2	2:T:13:A:C2	3.06	0.43
1:E:180:ILE:HA	1:E:184:TRP:CE3	2.53	0.43
1:C:8:SER:HB2	1:C:46:ALA:HB3	2.00	0.43
1:I:181:MET:CB	1:I:182:PRO:HD3	2.48	0.43
1:K:178:PRO:O	1:K:182:PRO:HG2	2.18	0.43
2:R:1:G:C5	2:R:19:A:C2	3.07	0.43
1:D:49:ILE:HD12	1:D:103:ILE:HD11	2.00	0.43
1:E:84:ARG:HD3	1:I:87:ILE:HD11	2.00	0.43
1:M:6:LEU:HD23	1:M:9:ALA:HA	2.00	0.43
1:D:46:ALA:HB2	1:D:99:LEU:HD21	1.99	0.43
1:G:30:VAL:HG22	1:G:61:SER:HB3	2.01	0.43
2:R:5:C:O2'	2:R:6:U:OP2	2.31	0.43
1:C:154:LEU:HD11	1:C:162:GLN:HG2	2.01	0.42
1:F:178:PRO:O	1:F:182:PRO:HG2	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:178:PRO:O	1:J:182:PRO:HG2	2.19	0.42
1:L:30:VAL:HG11	1:L:184:TRP:CZ3	2.54	0.42
1:L:132:TYR:CD1	1:L:142:ILE:HD12	2.54	0.42
2:Q:8:U:H2'	2:Q:10:C:C4	2.54	0.42
1:C:16:ASP:O	1:C:17:LEU:HG	2.19	0.42
2:R:4:G:OP2	2:R:4:G:C8	2.71	0.42
2:O:5:C:O2'	2:O:6:U:P	2.77	0.42
1:C:181:MET:HA	1:C:218:VAL:HG11	2.01	0.42
1:I:65:ALA:HA	1:I:112:TRP:HB2	2.02	0.42
2:R:20:C:C2	2:R:21:C:N3	2.87	0.42
1:A:116:LEU:HD23	1:A:179:ILE:HD11	2.00	0.42
1:G:68:LEU:HB2	1:G:112:TRP:CE2	2.54	0.42
1:E:87:ILE:HD11	1:I:80:ASP:CG	2.43	0.42
1:I:157:GLU:CD	1:I:160:VAL:HG11	2.44	0.42
2:P:3:G:O2'	2:P:4:G:H5'	2.20	0.42
2:T:3:G:C2'	2:T:4:G:H5'	2.50	0.42
1:D:29:THR:CG2	1:D:60:VAL:HG22	2.49	0.42
1:I:6:LEU:HD21	1:I:228:ARG:CZ	2.50	0.42
1:I:195:PRO:HA	1:I:223:LEU:HB2	2.02	0.42
1:L:149:PHE:CD2	1:L:169:CYS:SG	3.13	0.42
1:B:146:ILE:HG12	1:B:169:CYS:HB3	2.02	0.41
1:I:198:ILE:HD11	1:I:202:MET:HG3	2.02	0.41
2:P:3:G:C2'	2:P:4:G:H5'	2.50	0.41
2:P:20:C:C3'	2:P:21:C:H5''	2.50	0.41
1:F:16:ASP:HB3	1:F:222:PRO:HB2	2.01	0.41
2:P:20:C:C2'	2:P:21:C:H5''	2.50	0.41
1:E:195:PRO:HA	1:E:223:LEU:HB2	2.03	0.41
1:I:39:TYR:HA	1:I:44:LYS:HD2	2.01	0.41
1:B:77:THR:HG21	1:E:99:LEU:HD13	2.03	0.41
1:H:34:ALA:HB1	1:H:69:GLN:NE2	2.36	0.41
1:H:178:PRO:O	1:H:182:PRO:HG2	2.20	0.41
1:L:8:SER:HB2	1:L:46:ALA:CB	2.51	0.41
1:M:181:MET:CB	1:M:182:PRO:HD3	2.50	0.41
2:O:4:G:O2'	2:O:5:C:OP2	2.34	0.41
1:E:67:THR:HG1	1:E:112:TRP:HD1	1.68	0.41
1:K:116:LEU:HD23	1:K:179:ILE:HD11	2.03	0.41
1:B:172:TYR:CD1	1:B:172:TYR:C	2.98	0.41
1:C:45:LEU:O	1:C:49:ILE:HG12	2.21	0.41
1:K:45:LEU:O	1:K:48:THR:HB	2.21	0.41
1:M:138:TYR:CZ	1:M:142:ILE:HD11	2.56	0.41
1:B:181:MET:CB	1:B:182:PRO:HD3	2.51	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:THR:HG1	1:E:112:TRP:CD1	2.39	0.41
1:F:214:HIS:CG	1:F:217:ARG:NH1	2.88	0.41
1:M:132:TYR:CE1	1:M:139:ARG:HG3	2.55	0.41
1:A:77:THR:HG22	1:A:80:ASP:OD2	2.21	0.41
1:B:5:THR:HG23	1:B:5:THR:O	2.21	0.41
1:F:28:SER:HB2	1:F:189:PHE:HA	2.02	0.41
1:F:34:ALA:H	1:F:40:HIS:CE1	2.39	0.41
1:L:68:LEU:HG	1:L:172:TYR:CE2	2.56	0.41
1:M:34:ALA:H	1:M:40:HIS:CE1	2.38	0.41
2:O:3:G:C2'	2:O:4:G:H5'	2.50	0.41
2:Q:7:A:O2'	2:Q:8:U:O5'	2.38	0.41
1:I:6:LEU:HD23	1:I:9:ALA:HA	2.02	0.41
1:L:8:SER:HB2	1:L:46:ALA:HB3	2.02	0.41
1:L:30:VAL:HG22	1:L:61:SER:HB3	2.03	0.41
1:E:39:TYR:HA	1:E:44:LYS:HD2	2.02	0.40
1:K:77:THR:CG2	1:K:79:ILE:HG22	2.51	0.40
1:A:8:SER:HB2	1:A:46:ALA:HB3	2.04	0.40
1:I:214:HIS:CG	1:I:217:ARG:NH1	2.89	0.40
2:O:15:C:H2'	2:O:16:U:O4'	2.22	0.40
1:E:211:VAL:N	1:E:212:PRO:CD	2.84	0.40
1:B:149:PHE:HD2	1:B:169:CYS:SG	2.45	0.40
1:C:39:TYR:HA	1:C:44:LYS:HD2	2.03	0.40
1:F:181:MET:SD	1:F:206:ARG:HB2	2.61	0.40
1:K:146:ILE:HG12	1:K:169:CYS:HB3	2.04	0.40
1:L:132:TYR:HD1	1:L:142:ILE:HD12	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/248 (91%)	220 (98%)	5 (2%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	226/248 (91%)	221 (98%)	5 (2%)	0	100	100
1	C	225/248 (91%)	218 (97%)	7 (3%)	0	100	100
1	D	226/248 (91%)	221 (98%)	5 (2%)	0	100	100
1	E	225/248 (91%)	220 (98%)	5 (2%)	0	100	100
1	F	225/248 (91%)	220 (98%)	5 (2%)	0	100	100
1	G	225/248 (91%)	217 (96%)	8 (4%)	0	100	100
1	H	226/248 (91%)	220 (97%)	6 (3%)	0	100	100
1	I	225/248 (91%)	221 (98%)	4 (2%)	0	100	100
1	J	225/248 (91%)	219 (97%)	6 (3%)	0	100	100
1	K	225/248 (91%)	221 (98%)	4 (2%)	0	100	100
1	L	225/248 (91%)	220 (98%)	5 (2%)	0	100	100
1	M	225/248 (91%)	221 (98%)	4 (2%)	0	100	100
1	N	226/248 (91%)	221 (98%)	5 (2%)	0	100	100
All	All	3154/3472 (91%)	3080 (98%)	74 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/210 (92%)	193 (100%)	0	100	100
1	B	194/210 (92%)	194 (100%)	0	100	100
1	C	193/210 (92%)	193 (100%)	0	100	100
1	D	194/210 (92%)	194 (100%)	0	100	100
1	E	193/210 (92%)	193 (100%)	0	100	100
1	F	193/210 (92%)	193 (100%)	0	100	100
1	G	193/210 (92%)	193 (100%)	0	100	100
1	H	194/210 (92%)	194 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	193/210 (92%)	193 (100%)	0	100	100
1	J	193/210 (92%)	193 (100%)	0	100	100
1	K	193/210 (92%)	193 (100%)	0	100	100
1	L	193/210 (92%)	193 (100%)	0	100	100
1	M	193/210 (92%)	193 (100%)	0	100	100
1	N	194/210 (92%)	194 (100%)	0	100	100
All	All	2706/2940 (92%)	2706 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	108	ASN
1	B	56	ASN
1	B	96	ASN
1	B	130	HIS
1	B	214	HIS
1	C	40	HIS
1	C	82	HIS
1	D	11	HIS
1	D	40	HIS
1	D	186	HIS
1	E	82	HIS
1	E	130	HIS
1	E	214	HIS
1	G	108	ASN
1	H	108	ASN
1	I	40	HIS
1	I	130	HIS
1	K	69	GLN
1	K	108	ASN
1	L	69	GLN
1	L	108	ASN
1	M	82	HIS
1	M	130	HIS
1	M	162	GLN
1	N	69	GLN
1	N	130	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	N	214	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	O	20/22 (90%)	9 (45%)	0
2	P	20/22 (90%)	11 (55%)	0
2	Q	20/22 (90%)	10 (50%)	0
2	R	20/22 (90%)	10 (50%)	2 (10%)
2	T	20/22 (90%)	10 (50%)	0
All	All	100/110 (90%)	50 (50%)	2 (2%)

All (50) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	O	4	G
2	O	5	C
2	O	6	U
2	O	8	U
2	O	10	C
2	O	11	G
2	O	12	U
2	O	14	G
2	O	16	U
2	P	4	G
2	P	5	C
2	P	6	U
2	P	8	U
2	P	9	U
2	P	10	C
2	P	11	G
2	P	12	U
2	P	16	U
2	P	18	C
2	P	21	C
2	R	4	G
2	R	5	C
2	R	6	U
2	R	8	U
2	R	9	U
2	R	10	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	R	11	G
2	R	12	U
2	R	16	U
2	R	21	C
2	Q	4	G
2	Q	5	C
2	Q	6	U
2	Q	8	U
2	Q	9	U
2	Q	10	C
2	Q	11	G
2	Q	12	U
2	Q	16	U
2	Q	21	C
2	T	4	G
2	T	5	C
2	T	6	U
2	T	8	U
2	T	10	C
2	T	11	G
2	T	12	U
2	T	14	G
2	T	16	U
2	T	21	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	R	11	G
2	R	20	C

## 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

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	227/248 (91%)	-0.51	0	100	100	52, 86, 137, 160	0
1	B	228/248 (91%)	-0.53	0	100	100	51, 85, 141, 162	0
1	C	227/248 (91%)	-0.44	0	100	100	61, 101, 154, 167	0
1	D	228/248 (91%)	-0.44	0	100	100	60, 99, 165, 185	0
1	E	227/248 (91%)	-0.49	0	100	100	54, 93, 145, 185	0
1	F	227/248 (91%)	-0.28	1 (0%)	88	71	70, 118, 174, 190	0
1	G	227/248 (91%)	-0.49	0	100	100	64, 98, 149, 180	0
1	H	228/248 (91%)	-0.35	0	100	100	88, 137, 181, 197	0
1	I	227/248 (91%)	-0.43	0	100	100	70, 118, 164, 180	0
1	J	227/248 (91%)	-0.28	0	100	100	86, 128, 175, 198	0
1	K	227/248 (91%)	-0.41	0	100	100	89, 129, 171, 190	0
1	L	227/248 (91%)	-0.32	0	100	100	84, 113, 164, 186	0
1	M	227/248 (91%)	-0.27	0	100	100	97, 129, 171, 191	0
1	N	228/248 (91%)	-0.24	0	100	100	94, 134, 174, 192	0
2	O	21/22 (95%)	-0.39	0	100	100	85, 108, 119, 140	9 (42%)
2	P	21/22 (95%)	-0.44	0	100	100	98, 107, 130, 135	4 (19%)
2	Q	21/22 (95%)	-0.28	0	100	100	128, 155, 170, 177	0
2	R	21/22 (95%)	0.31	0	100	100	110, 149, 182, 189	15 (71%)
2	T	21/22 (95%)	0.01	0	100	100	153, 169, 197, 215	9 (42%)
All	All	3287/3582 (91%)	-0.38	1 (0%)	100	100	51, 114, 170, 215	37 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	73	LEU	2.2

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.