



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:30 AM UTC

PDB ID : 2PY9 / pdb_00002py9
Title : Protein-RNA Interaction involving KH1 domain from Human Poly(C)-Binding Protein-2
Authors : James, T.L.; Du, Z.; Lee, J.K.
Deposited on : 2007-05-15
Resolution : 2.56 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

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

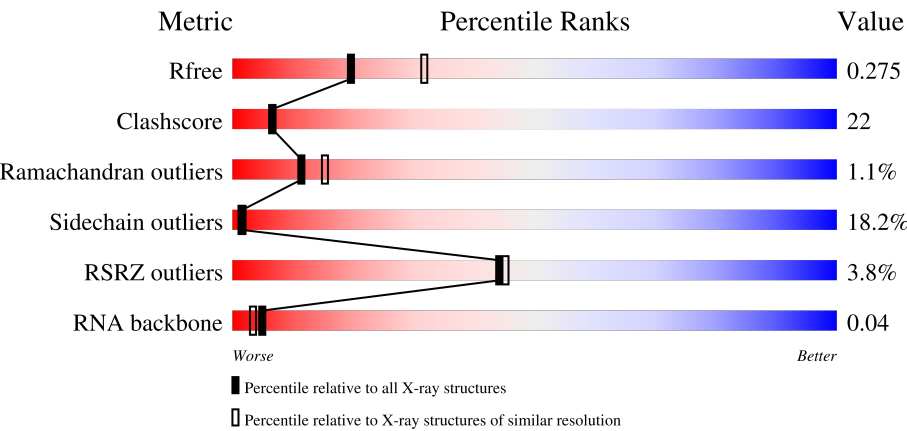
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)
RNA backbone	3983	1013 (2.80-2.32)

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	E	12	8% 50% 50%
1	F	12	8% 58% 33%
2	A	73	3% 41% 45% 8% • •
2	B	73	% 47% 32% 12% • 5%

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Mol	Chain	Length	Quality of chain
2	C	73	3% 51% 32% 12% 5%
2	D	73	7% 51% 32% 8% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2669 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 RNA chain called 12-mer C-rich strand of human telomeric RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	12	Total	C	N	O	P	0	0	0
			245	112	42	80	11			
1	F	12	Total	C	N	O	P	0	0	0
			245	112	42	80	11			

- Molecule 2 is a protein called Poly(rC)-binding protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	72	Total	C	N	O	S	Se	0	0	0
			550	346	98	102	1	3			
2	B	69	Total	C	N	O	S	Se	0	0	0
			526	331	93	98	1	3			
2	C	69	Total	C	N	O	S	Se	0	0	0
			526	331	93	98	1	3			
2	D	69	Total	C	N	O	S	Se	0	0	0
			526	331	93	98	1	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	LYS	-	cloning artifact	UNP Q15366
A	20	MSE	MET	modified residue	UNP Q15366
A	39	MSE	MET	modified residue	UNP Q15366
A	74	MSE	MET	modified residue	UNP Q15366
B	10	LYS	-	cloning artifact	UNP Q15366
B	20	MSE	MET	modified residue	UNP Q15366
B	39	MSE	MET	modified residue	UNP Q15366
B	74	MSE	MET	modified residue	UNP Q15366
C	10	LYS	-	cloning artifact	UNP Q15366
C	20	MSE	MET	modified residue	UNP Q15366
C	39	MSE	MET	modified residue	UNP Q15366
C	74	MSE	MET	modified residue	UNP Q15366
D	10	LYS	-	cloning artifact	UNP Q15366

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Chain	Residue	Modelled	Actual	Comment	Reference
D	20	MSE	MET	modified residue	UNP Q15366
D	39	MSE	MET	modified residue	UNP Q15366
D	74	MSE	MET	modified residue	UNP Q15366

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	3	Total O 3 3	0	0
3	F	4	Total O 4 4	0	0
3	A	9	Total O 9 9	0	0
3	B	14	Total O 14 14	0	0
3	C	11	Total O 11 11	0	0
3	D	10	Total O 10 10	0	0

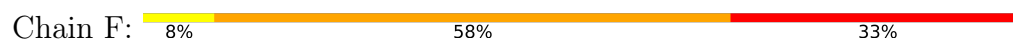
3 Residue-property plots [i](#)

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.

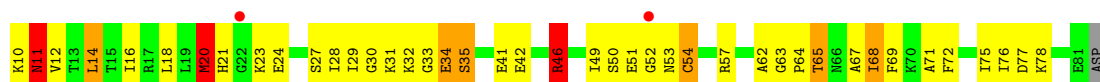
- Molecule 1: 12-mer C-rich strand of human telomeric RNA



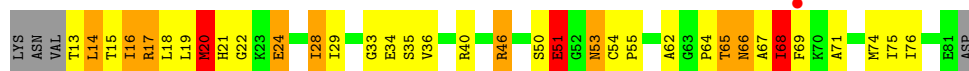
- Molecule 1: 12-mer C-rich strand of human telomeric RNA



- Molecule 2: Poly(rC)-binding protein 2



- Molecule 2: Poly(rC)-binding protein 2

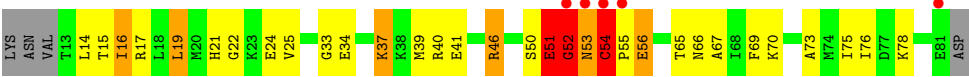


- Molecule 2: Poly(rC)-binding protein 2



- Molecule 2: Poly(rC)-binding protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	92.01Å 58.70Å 71.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.56 40.00 – 2.56	Depositor EDS
% Data completeness (in resolution range)	94.2 (40.00-2.56) 94.2 (40.00-2.56)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.218 , 0.269 0.234 , 0.275	Depositor DCC
R_{free} test set	591 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2669	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.59% 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

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	E	1.83	7/272 (2.6%)	2.91	41/420 (9.8%)
1	F	1.63	3/272 (1.1%)	2.85	39/420 (9.3%)
2	A	1.86	9/551 (1.6%)	1.70	11/729 (1.5%)
2	B	1.80	10/527 (1.9%)	1.83	18/697 (2.6%)
2	C	1.72	4/527 (0.8%)	1.84	18/697 (2.6%)
2	D	1.79	5/527 (0.9%)	1.90	14/697 (2.0%)
All	All	1.78	38/2676 (1.4%)	2.11	141/3660 (3.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	16	ILE	CA-CB	7.92	1.67	1.55
1	E	8	A	O5'-C5'	7.69	1.54	1.42
1	E	2	A	O5'-C5'	6.95	1.53	1.42
2	D	16	ILE	C-O	6.92	1.31	1.24
1	E	9	C	C3'-O3'	6.88	1.53	1.43
2	A	46	ARG	CZ-NH2	-6.87	1.24	1.33
1	F	10	C	C1'-N1	6.83	1.57	1.47
2	B	46	ARG	CZ-NH2	-6.50	1.25	1.33
2	D	51	GLU	CA-C	-6.34	1.44	1.52
2	D	51	GLU	CB-CG	-6.24	1.33	1.52
2	B	71	ALA	CA-CB	-6.12	1.43	1.53
2	A	71	ALA	C-O	-5.96	1.17	1.24
2	A	30	GLY	N-CA	5.94	1.51	1.45
2	B	67	ALA	N-CA	-5.92	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	46	ARG	CB-CG	-5.88	1.34	1.52
1	F	12	U	O5'-C5'	5.84	1.51	1.42
2	A	75	ILE	CA-CB	5.82	1.61	1.54
1	E	2	A	P-O5'	5.75	1.68	1.59
1	E	3	C	C3'-O3'	-5.70	1.34	1.43
2	C	68	ILE	CG1-CD1	-5.68	1.29	1.51
2	B	75	ILE	CA-CB	5.65	1.61	1.54
2	B	65	THR	CA-C	5.62	1.60	1.52
2	A	20	MSE	CA-C	5.61	1.59	1.52
1	E	12	U	C1'-N1	5.57	1.55	1.47
2	C	67	ALA	N-CA	-5.55	1.39	1.46
1	F	12	U	C1'-N1	5.45	1.55	1.47
2	C	52	GLY	N-CA	-5.45	1.40	1.45
2	A	42	GLU	CA-C	-5.38	1.45	1.52
2	B	17	ARG	CA-C	5.35	1.59	1.52
2	C	25	VAL	CA-CB	5.35	1.61	1.54
2	A	41	GLU	CG-CD	5.25	1.65	1.52
2	B	46	ARG	CA-C	-5.24	1.46	1.52
1	E	11	C	C1'-N1	5.14	1.56	1.48
2	A	54	CYS	CB-SG	-5.07	1.64	1.81
2	B	71	ALA	CA-C	-5.07	1.46	1.52
2	D	25	VAL	CA-C	-5.02	1.47	1.52
2	A	63	GLY	C-O	5.01	1.30	1.24
2	B	74	MSE	SE-CE	5.01	2.10	1.95

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	10	C	O4'-C1'-C2'	-14.44	91.36	105.80
1	F	6	U	C1'-C2'-O2'	-13.03	92.25	111.80
1	F	9	C	C1'-C2'-O2'	-11.73	94.20	111.80
1	F	4	C	C4'-C3'-C2'	-11.26	91.34	102.60
1	E	11	C	C4'-C3'-C2'	-10.76	91.84	102.60
1	E	2	A	C3'-C2'-C1'	-9.72	91.78	101.50
1	F	4	C	O4'-C1'-C2'	-9.38	96.42	105.80
1	F	7	A	C5'-C4'-O4'	9.16	122.84	109.10
1	E	5	C	C3'-C2'-C1'	8.73	110.03	101.30
1	E	1	A	C3'-C2'-C1'	-8.58	92.92	101.50
1	E	11	C	N1-C1'-C2'	8.45	124.67	112.00
2	D	54	CYS	CA-C-N	-8.40	112.26	120.83
2	D	54	CYS	C-N-CA	-8.40	112.26	120.83
1	E	2	A	P-O5'-C5'	8.18	133.17	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	4	C	O4'-C1'-N1	8.15	120.42	108.20
1	F	10	C	C1'-C2'-O2'	-8.13	99.61	111.80
1	E	11	C	O4'-C1'-C2'	-8.12	99.48	107.60
1	F	10	C	C3'-C2'-O2'	-8.03	102.55	114.60
1	F	4	C	C2'-C3'-O3'	7.96	121.43	109.50
1	F	5	C	O3'-P-O5'	7.92	115.88	104.00
2	D	56	GLU	CA-CB-CG	-7.90	98.30	114.10
2	B	53	ASN	N-CA-C	-7.87	100.05	111.30
2	B	15	THR	CA-C-N	-7.85	112.23	123.06
2	B	15	THR	C-N-CA	-7.85	112.23	123.06
1	E	4	C	C1'-C2'-O2'	-7.72	100.22	111.80
1	F	3	C	C1'-C2'-O2'	-7.68	100.28	111.80
2	A	68	ILE	CB-CA-C	-7.60	101.97	111.70
2	D	67	ALA	N-CA-C	-7.39	102.92	112.23
2	B	20	MSE	N-CA-C	7.38	121.75	108.69
1	E	11	C	O5'-C5'-C4'	-7.37	100.44	111.50
1	E	9	C	C4'-C3'-C2'	-7.26	95.34	102.60
1	F	12	U	P-O5'-C5'	7.20	131.69	120.90
2	B	46	ARG	CB-CG-CD	-7.12	94.92	111.30
1	F	11	C	C1'-C2'-O2'	-6.97	97.95	108.40
1	E	9	C	C2'-C3'-O3'	6.96	119.94	109.50
1	E	1	A	N9-C1'-C2'	6.96	124.43	114.00
1	F	11	C	O4'-C1'-N1	6.91	118.86	108.50
2	C	42	GLU	N-CA-C	6.89	119.64	111.71
2	C	56	GLU	N-CA-CB	-6.88	100.32	110.37
1	E	2	A	O4'-C1'-N9	6.86	118.50	108.20
1	F	9	C	O4'-C1'-C2'	-6.86	98.94	105.80
2	C	68	ILE	CB-CA-C	-6.83	103.14	111.88
2	C	46	ARG	NE-CZ-NH2	6.81	125.33	119.20
1	E	5	C	C5'-C4'-C3'	-6.70	105.94	116.00
1	F	11	C	N1-C1'-C2'	-6.69	101.96	112.00
1	E	1	A	P-O3'-C3'	6.65	130.17	120.20
2	A	20	MSE	N-CA-C	6.64	120.32	109.24
2	C	55	PRO	N-CA-C	-6.60	106.28	114.20
2	C	54	CYS	N-CA-C	6.59	119.00	109.84
2	B	46	ARG	CB-CA-C	-6.59	99.10	109.84
1	E	10	C	O5'-P-OP2	-6.55	88.34	108.00
1	E	9	C	O3'-P-O5'	6.50	113.76	104.00
2	A	46	ARG	NE-CZ-NH2	6.47	125.03	119.20
2	D	55	PRO	N-CA-C	-6.46	107.96	114.68
2	C	46	ARG	NE-CZ-NH1	-6.32	115.18	121.50
1	F	3	C	O5'-C5'-C4'	-6.29	102.27	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	9	C	C3'-C2'-C1'	6.29	107.79	101.50
1	E	7	A	O3'-P-O5'	-6.26	94.60	104.00
1	F	11	C	C3'-C2'-C1'	6.15	107.45	101.30
1	E	7	A	C2'-C3'-O3'	6.15	118.72	109.50
1	E	10	C	C5'-C4'-O4'	-6.14	99.89	109.10
2	A	51	GLU	N-CA-C	6.13	117.95	110.41
1	E	10	C	C1'-O4'-C4'	6.08	115.78	109.70
1	E	2	A	O4'-C4'-C3'	-6.06	100.04	106.10
1	F	12	U	C5'-C4'-O4'	6.04	118.16	109.10
1	F	8	A	P-O3'-C3'	6.02	129.23	120.20
1	E	7	A	O4'-C1'-C2'	-6.00	99.80	105.80
1	E	10	C	C3'-C2'-O2'	-5.99	105.61	114.60
1	E	9	C	C5'-C4'-O4'	5.99	118.08	109.10
2	B	66	ASN	N-CA-C	5.92	118.69	111.82
2	B	51	GLU	CB-CG-CD	-5.92	102.54	112.60
1	F	11	C	OP1-P-OP2	5.91	137.33	119.60
2	B	50	SER	CA-C-N	5.88	129.18	120.95
2	B	50	SER	C-N-CA	5.88	129.18	120.95
2	D	51	GLU	N-CA-CB	5.88	119.22	110.29
1	E	1	A	C1'-C2'-O2'	5.88	120.61	111.80
2	B	69	PHE	CB-CA-C	-5.84	100.74	110.68
1	F	2	A	C3'-C2'-O2'	-5.83	105.85	114.60
2	D	66	ASN	N-CA-C	-5.81	106.19	113.28
1	E	5	C	O3'-P-O5'	5.77	112.66	104.00
2	A	69	PHE	N-CA-C	5.76	118.30	111.33
2	C	63	GLY	CA-C-N	-5.76	113.76	119.92
2	C	63	GLY	C-N-CA	-5.76	113.76	119.92
1	E	12	U	C5'-C4'-O4'	5.73	117.69	109.10
2	A	35	SER	CB-CA-C	-5.68	99.11	110.42
1	E	8	A	C4'-C3'-O3'	-5.66	100.91	109.40
2	C	69	PHE	N-CA-C	5.61	117.84	111.11
1	F	10	C	O5'-C5'-C4'	-5.59	103.31	111.70
1	F	11	C	C4'-C3'-O3'	-5.59	104.61	113.00
1	F	11	C	C3'-C2'-O2'	5.57	119.06	110.70
2	A	78	LYS	CD-CE-NZ	-5.56	94.10	111.90
1	F	6	U	C3'-C2'-C1'	5.55	107.05	101.50
2	B	46	ARG	NE-CZ-NH1	5.55	127.05	121.50
2	A	51	GLU	N-CA-CB	-5.55	102.78	110.38
2	A	77	ASP	N-CA-CB	-5.53	100.71	110.39
1	E	1	A	O4'-C4'-C3'	-5.50	100.60	106.10
2	D	50	SER	CA-C-N	-5.49	112.28	121.39
2	D	50	SER	C-N-CA	-5.49	112.28	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2	A	O3'-P-O5'	-5.43	95.86	104.00
1	E	12	U	O4'-C1'-N1	5.42	116.33	108.20
2	A	67	ALA	N-CA-C	-5.41	105.39	111.28
1	E	3	C	O3'-P-O5'	5.39	112.09	104.00
1	F	12	U	O4'-C1'-C2'	-5.38	100.42	105.80
1	F	8	A	C2'-C3'-O3'	5.37	117.56	109.50
1	E	9	C	C3'-C2'-O2'	-5.36	106.56	114.60
1	F	2	A	O4'-C1'-C2'	-5.33	100.47	105.80
1	F	4	C	C1'-C2'-O2'	-5.33	103.80	111.80
2	D	25	VAL	N-CA-C	-5.33	107.22	111.81
1	E	1	A	C4'-C3'-C2'	-5.33	97.27	102.60
2	B	69	PHE	N-CA-C	5.33	117.78	111.33
2	A	46	ARG	CD-NE-CZ	-5.33	116.94	124.40
2	C	51	GLU	CA-C-N	-5.33	115.49	122.63
2	C	51	GLU	C-N-CA	-5.33	115.49	122.63
2	C	56	GLU	CB-CA-C	-5.29	104.17	110.94
2	C	60	THR	CA-C-N	-5.28	115.71	123.00
2	C	60	THR	C-N-CA	-5.28	115.71	123.00
1	E	10	C	C4'-C3'-O3'	5.27	117.30	109.40
1	F	3	C	O3'-P-O5'	5.23	111.85	104.00
2	D	34	GLU	CB-CA-C	-5.21	102.47	110.81
2	C	75	ILE	N-CA-C	-5.21	105.63	110.53
2	D	69	PHE	N-CA-C	5.20	116.64	111.07
1	E	3	C	O4'-C1'-C2'	-5.20	100.60	105.80
1	F	7	A	C3'-C2'-O2'	-5.19	106.82	114.60
1	E	6	U	O5'-C5'-C4'	-5.18	103.92	111.70
2	B	51	GLU	N-CA-C	5.18	117.73	109.96
2	D	22	GLY	N-CA-C	-5.16	106.48	113.24
1	F	5	C	N1-C1'-C2'	5.11	119.67	112.00
2	D	37	LYS	CG-CD-CE	-5.11	99.56	111.30
2	C	50	SER	CA-C-N	-5.09	113.99	122.64
2	C	50	SER	C-N-CA	-5.09	113.99	122.64
1	F	4	C	P-O5'-C5'	-5.08	113.29	120.90
1	E	6	U	O4'-C1'-C2'	-5.07	100.73	105.80
1	F	4	C	C5'-C4'-C3'	-5.07	107.59	115.20
1	F	6	U	O4'-C1'-N1	5.06	115.80	108.20
2	B	68	ILE	CB-CA-C	-5.06	105.49	111.97
2	B	34	GLU	N-CA-CB	-5.06	102.69	110.12
2	B	54	CYS	N-CA-CB	-5.04	101.79	110.01
1	E	7	A	C3'-C2'-C1'	5.04	106.54	101.50
2	B	51	GLU	N-CA-CB	-5.04	102.34	109.85
1	E	9	C	O5'-P-OP2	5.03	123.10	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	10	C	O4'-C1'-C2'	-5.01	100.79	105.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	52	GLY	Peptide
2	D	53	ASN	Peptide

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	E	245	0	132	10	0
1	F	245	0	132	9	0
2	A	550	0	588	31	0
2	B	526	0	560	22	0
2	C	526	0	560	27	0
2	D	526	0	560	24	0
3	A	9	0	0	3	0
3	B	14	0	0	1	0
3	C	11	0	0	3	0
3	D	10	0	0	2	0
3	E	3	0	0	0	0
3	F	4	0	0	0	0
All	All	2669	0	2532	111	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 22.

All (111) 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)
2:A:46:ARG:HH11	2:A:46:ARG:CG	1.64	1.10
2:A:46:ARG:HH11	2:A:46:ARG:HG2	0.87	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:56:GLU:HB3	3:C:86:HOH:O	1.57	1.02
2:A:46:ARG:HG2	2:A:46:ARG:NH1	1.65	1.00
2:A:18:LEU:HD23	2:B:18:LEU:HD23	1.45	0.97
2:D:46:ARG:HH11	2:D:46:ARG:HG2	1.30	0.96
2:A:46:ARG:CG	2:A:46:ARG:NH1	2.26	0.86
2:D:39:MSE:HE1	2:D:75:ILE:HG12	1.60	0.82
2:D:39:MSE:CE	2:D:75:ILE:HG13	2.09	0.82
2:D:39:MSE:HE3	2:D:75:ILE:HG13	1.63	0.81
2:A:18:LEU:CD2	2:B:18:LEU:HD23	2.13	0.77
2:D:39:MSE:HE1	2:D:75:ILE:CG1	2.14	0.77
1:F:4:C:O5'	1:F:4:C:H2'	1.86	0.75
2:D:56:GLU:HG3	2:D:56:GLU:O	1.86	0.74
2:D:39:MSE:CE	2:D:75:ILE:CG1	2.65	0.74
2:B:51:GLU:OE2	2:B:51:GLU:HA	1.85	0.73
1:F:11:C:H2'	1:F:12:U:C6	2.25	0.72
1:E:6:U:O2'	1:E:7:A:C8	2.43	0.71
2:A:20:MSE:HA	3:A:87:HOH:O	1.92	0.69
2:B:29:ILE:HG23	2:B:33:GLY:HA2	1.74	0.69
2:A:11:ASN:HB3	3:A:83:HOH:O	1.93	0.69
1:F:4:C:H4'	1:F:5:C:H5'	1.77	0.67
2:C:76:ILE:CG2	2:D:65:THR:HG23	2.24	0.67
2:D:46:ARG:HH11	2:D:46:ARG:CG	2.04	0.66
2:C:20:MSE:HE2	2:C:28:ILE:CD1	2.25	0.66
2:C:55:PRO:HD2	3:C:86:HOH:O	1.96	0.65
1:E:3:C:H2'	1:E:3:C:OP1	1.97	0.65
2:B:29:ILE:CG2	2:B:33:GLY:HA2	2.27	0.65
2:C:54:CYS:C	2:C:56:GLU:H	2.05	0.64
1:E:7:A:O2'	1:E:8:A:C8	2.48	0.64
1:E:8:A:H1'	1:E:9:C:H5'	1.79	0.63
2:A:53:ASN:N	3:A:90:HOH:O	2.31	0.63
2:C:43:SER:HB3	2:C:74:MSE:CE	2.30	0.62
2:A:10:LYS:O	2:A:10:LYS:HG3	2.00	0.61
2:B:20:MSE:HE1	2:B:28:ILE:CD1	2.31	0.61
2:B:17:ARG:HD2	3:B:92:HOH:O	2.00	0.61
2:C:36:VAL:HG23	2:C:39:MSE:HE2	1.82	0.60
2:C:20:MSE:HG3	2:C:59:ILE:HG13	1.83	0.60
2:A:21:HIS:HB2	2:A:24:GLU:HG3	1.84	0.60
2:D:40:ARG:HG2	3:D:84:HOH:O	2.02	0.60
2:C:16:ILE:HD12	2:C:17:ARG:N	2.18	0.59
2:B:21:HIS:HB2	2:B:24:GLU:HG3	1.85	0.58
2:A:46:ARG:NH1	2:A:46:ARG:CB	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:72:PHE:CE1	2:C:76:ILE:CD1	2.86	0.58
1:E:11:C:H2'	1:E:12:U:H5'	1.85	0.58
2:B:19:LEU:C	2:B:20:MSE:HG2	2.30	0.57
2:C:19:LEU:HB2	2:D:19:LEU:HD12	1.85	0.57
2:C:72:PHE:CZ	2:C:76:ILE:CD1	2.88	0.56
2:A:46:ARG:CB	2:A:46:ARG:CZ	2.80	0.56
1:E:5:C:O2'	1:E:6:U:H5'	2.06	0.55
2:C:72:PHE:CZ	2:C:76:ILE:HD11	2.42	0.55
2:A:18:LEU:HD23	2:B:18:LEU:CD2	2.30	0.54
2:A:29:ILE:HG22	2:A:33:GLY:HA2	1.89	0.54
2:B:51:GLU:OE2	2:B:51:GLU:CA	2.50	0.54
2:D:78:LYS:HE2	3:D:92:HOH:O	2.08	0.54
2:D:53:ASN:HB3	2:D:54:CYS:HA	1.89	0.54
2:C:76:ILE:CG2	2:D:65:THR:CG2	2.88	0.51
2:A:52:GLY:C	2:A:54:CYS:H	2.19	0.51
1:F:1:A:H5'	1:F:1:A:N3	2.26	0.51
2:C:76:ILE:HG23	2:D:65:THR:HG23	1.93	0.50
1:E:11:C:C2'	1:E:12:U:H5'	2.42	0.50
2:A:18:LEU:CD2	2:B:18:LEU:CD2	2.87	0.49
2:A:20:MSE:HE3	2:A:24:GLU:HB2	1.95	0.48
1:F:1:A:O2'	1:F:2:A:P	2.71	0.48
1:F:10:C:N3	2:A:57:ARG:NH1	2.59	0.48
2:D:51:GLU:O	2:D:52:GLY:C	2.55	0.48
2:A:46:ARG:NH1	2:A:46:ARG:HB3	2.29	0.47
1:E:8:A:C2	1:E:9:C:C2	3.02	0.47
2:C:16:ILE:HD12	2:C:16:ILE:C	2.39	0.47
2:C:20:MSE:HE2	2:C:28:ILE:HD12	1.97	0.47
2:D:54:CYS:C	2:D:56:GLU:H	2.22	0.47
2:A:31:LYS:O	2:A:34:GLU:HG2	2.14	0.46
2:B:22:GLY:N	2:B:55:PRO:O	2.48	0.46
1:F:2:A:C3'	1:F:3:C:H5''	2.45	0.46
2:D:33:GLY:O	2:D:37:LYS:HB2	2.16	0.46
2:D:51:GLU:O	2:D:52:GLY:O	2.32	0.46
2:D:65:THR:O	2:D:65:THR:HG22	2.16	0.46
2:B:14:LEU:O	2:B:62:ALA:HA	2.15	0.45
2:C:20:MSE:CE	2:C:28:ILE:HD11	2.46	0.45
2:C:43:SER:HB3	2:C:74:MSE:HE1	1.98	0.45
1:E:4:C:H4'	1:E:5:C:H5'	1.98	0.45
2:C:69:PHE:HZ	2:D:73:ALA:HA	1.82	0.45
2:C:20:MSE:HE2	2:C:28:ILE:HD11	1.97	0.45
2:A:28:ILE:O	2:A:35:SER:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:64:PRO:O	2:A:65:THR:C	2.61	0.44
2:B:24:GLU:O	2:B:28:ILE:HD12	2.17	0.44
1:F:4:C:O5'	1:F:4:C:C2'	2.63	0.44
2:B:36:VAL:O	2:B:40:ARG:HG3	2.17	0.44
2:A:72:PHE:CE2	2:B:16:ILE:HD13	2.54	0.43
2:A:20:MSE:HE3	2:A:20:MSE:HB3	1.59	0.43
2:B:14:LEU:HB2	2:B:68:ILE:HD11	2.00	0.43
2:D:52:GLY:O	2:D:54:CYS:HB2	2.19	0.42
2:C:43:SER:HB3	2:C:74:MSE:HE3	1.99	0.42
2:A:29:ILE:CG2	2:A:33:GLY:HA2	2.50	0.42
2:A:12:VAL:O	2:A:64:PRO:HA	2.19	0.42
2:C:56:GLU:CB	3:C:86:HOH:O	2.37	0.42
2:C:37:LYS:HE2	2:C:37:LYS:HB2	1.52	0.42
2:D:53:ASN:N	2:D:54:CYS:HB2	2.35	0.42
2:A:20:MSE:HE1	2:A:28:ILE:HD12	2.03	0.41
2:B:20:MSE:HE3	2:B:24:GLU:HB2	2.03	0.41
2:A:14:LEU:O	2:A:62:ALA:HA	2.20	0.41
2:D:21:HIS:N	2:D:24:GLU:OE2	2.51	0.41
2:C:14:LEU:HD12	2:C:14:LEU:HA	1.93	0.41
2:B:64:PRO:O	2:B:65:THR:C	2.64	0.40
2:C:72:PHE:CE1	2:C:76:ILE:HD12	2.56	0.40
1:F:9:C:N4	2:A:27:SER:HB3	2.37	0.40
2:B:20:MSE:HE3	2:B:20:MSE:HB3	1.61	0.40
2:C:54:CYS:C	2:C:56:GLU:N	2.68	0.40
1:E:5:C:O2'	1:E:6:U:C5'	2.68	0.40
2:A:49:ILE:O	2:A:50:SER:C	2.65	0.40
2:B:21:HIS:O	2:B:24:GLU:HG3	2.22	0.40

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	
2	A	70/73 (96%)	63 (90%)	5 (7%)	2 (3%)	3	3
2	B	67/73 (92%)	64 (96%)	3 (4%)	0	100	100
2	C	67/73 (92%)	63 (94%)	4 (6%)	0	100	100
2	D	67/73 (92%)	60 (90%)	6 (9%)	1 (2%)	8	10
All	All	271/292 (93%)	250 (92%)	18 (7%)	3 (1%)	11	15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	52	GLY
2	A	11	ASN
2	A	65	THR

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	
2	A	60/58 (103%)	50 (83%)	10 (17%)	2	2
2	B	57/58 (98%)	44 (77%)	13 (23%)	1	1
2	C	57/58 (98%)	49 (86%)	8 (14%)	3	3
2	D	57/58 (98%)	46 (81%)	11 (19%)	1	1
All	All	231/232 (100%)	189 (82%)	42 (18%)	2	1

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	11	ASN
2	A	14	LEU
2	A	16	ILE
2	A	20	MSE
2	A	23	LYS
2	A	32	LYS
2	A	34	GLU
2	A	46	ARG

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Mol	Chain	Res	Type
2	A	68	ILE
2	A	76	ILE
2	B	13	THR
2	B	14	LEU
2	B	16	ILE
2	B	20	MSE
2	B	24	GLU
2	B	28	ILE
2	B	35	SER
2	B	46	ARG
2	B	51	GLU
2	B	53	ASN
2	B	66	ASN
2	B	68	ILE
2	B	76	ILE
2	C	14	LEU
2	C	16	ILE
2	C	17	ARG
2	C	37	LYS
2	C	41	GLU
2	C	70	LYS
2	C	76	ILE
2	C	80	GLU
2	D	14	LEU
2	D	15	THR
2	D	16	ILE
2	D	17	ARG
2	D	19	LEU
2	D	41	GLU
2	D	46	ARG
2	D	51	GLU
2	D	54	CYS
2	D	70	LYS
2	D	76	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	11	ASN
2	B	53	ASN
2	B	66	ASN
2	D	53	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	12/12 (100%)	8 (66%)	3 (25%)
1	F	12/12 (100%)	6 (50%)	2 (16%)
All	All	24/24 (100%)	14 (58%)	5 (20%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	2	A
1	E	3	C
1	E	4	C
1	E	5	C
1	E	7	A
1	E	8	A
1	E	9	C
1	E	10	C
1	F	2	A
1	F	4	C
1	F	7	A
1	F	8	A
1	F	9	C
1	F	10	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	1	A
1	E	2	A
1	E	3	C
1	F	1	A
1	F	9	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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 [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, 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	E	12/12 (100%)	0.25	1 (8%) 17 17	39, 52, 76, 81	0
1	F	12/12 (100%)	0.08	0 100 100	44, 48, 63, 82	0
2	A	69/73 (94%)	0.19	2 (2%) 53 55	18, 31, 47, 56	0
2	B	66/73 (90%)	0.05	1 (1%) 72 73	19, 31, 45, 60	0
2	C	66/73 (90%)	0.05	2 (3%) 52 54	21, 33, 49, 57	0
2	D	66/73 (90%)	0.21	5 (7%) 20 19	23, 34, 49, 63	0
All	All	291/316 (92%)	0.13	11 (3%) 44 45	18, 33, 53, 82	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	53	ASN	5.2
2	C	53	ASN	3.3
2	D	52	GLY	2.9
2	D	81	GLU	2.7
2	B	69	PHE	2.5
2	D	54	CYS	2.4
2	D	55	PRO	2.3
2	A	52	GLY	2.1
1	E	1	A	2.1
2	C	41	GLU	2.0
2	A	22	GLY	2.0

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.