Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:23 PM GMT

PDB ID	:	3TRZ
Title	:	Mouse Lin28A in complex with let-7d microRNA pre-element
Authors	:	Nam, Y.; Sliz, P.
Deposited on	:	2011-09-11
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

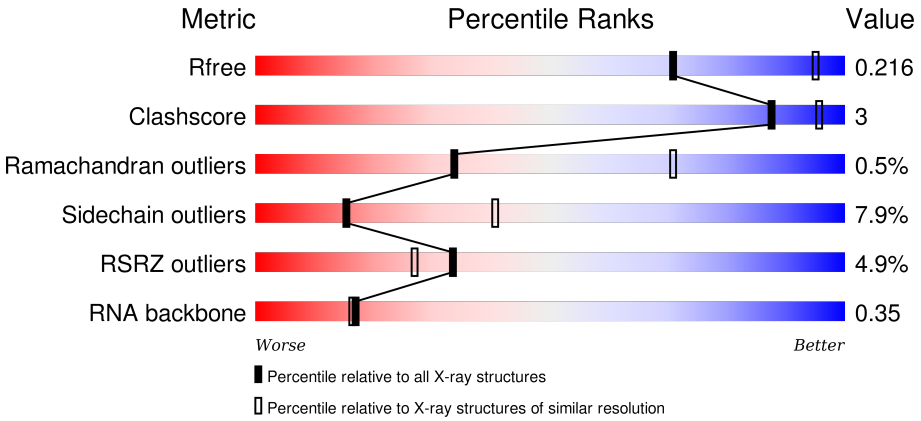
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	148	3% 74% 11% • 12%
1	B	148	6% 74% 12% • 12%
1	C	148	3% 78% 9% • 12%
1	D	148	4% 80% 6% • 12%

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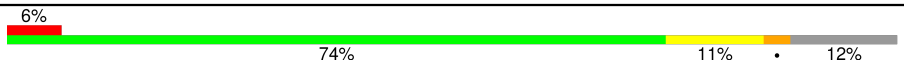
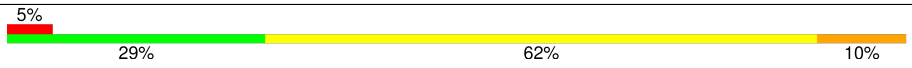
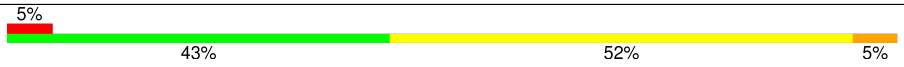
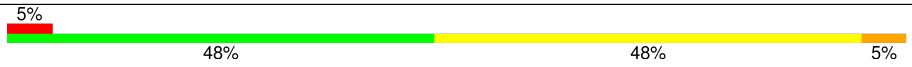
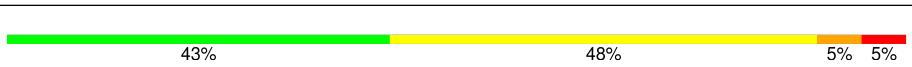
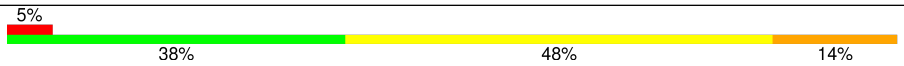
Mol	Chain	Length	Quality of chain
1	E	148	
1	F	148	
2	U	21	
2	V	21	
2	W	21	
2	X	21	
2	Y	21	
2	Z	21	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8694 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 Protein lin-28 homolog A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			994	631	179	172	12			
1	B	130	Total	C	N	O	S	0	0	0
			994	631	179	172	12			
1	C	130	Total	C	N	O	S	0	0	0
			994	631	179	172	12			
1	D	130	Total	C	N	O	S	0	0	0
			994	631	179	172	12			
1	E	130	Total	C	N	O	S	0	0	0
			994	631	179	172	12			
1	F	130	Total	C	N	O	S	0	0	0
			994	631	179	172	12			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	DELETION	UNP Q8K3Y3
A	?	-	ASN	DELETION	UNP Q8K3Y3
A	?	-	MET	DELETION	UNP Q8K3Y3
A	?	-	GLN	DELETION	UNP Q8K3Y3
A	?	-	LYS	DELETION	UNP Q8K3Y3
A	?	-	ARG	DELETION	UNP Q8K3Y3
A	?	-	ARG	DELETION	UNP Q8K3Y3
A	?	-	SER	DELETION	UNP Q8K3Y3
A	?	-	LYS	DELETION	UNP Q8K3Y3
B	?	-	LYS	DELETION	UNP Q8K3Y3
B	?	-	ASN	DELETION	UNP Q8K3Y3
B	?	-	MET	DELETION	UNP Q8K3Y3
B	?	-	GLN	DELETION	UNP Q8K3Y3
B	?	-	LYS	DELETION	UNP Q8K3Y3
B	?	-	ARG	DELETION	UNP Q8K3Y3
B	?	-	ARG	DELETION	UNP Q8K3Y3
B	?	-	SER	DELETION	UNP Q8K3Y3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	DELETION	UNP Q8K3Y3
C	?	-	LYS	DELETION	UNP Q8K3Y3
C	?	-	ASN	DELETION	UNP Q8K3Y3
C	?	-	MET	DELETION	UNP Q8K3Y3
C	?	-	GLN	DELETION	UNP Q8K3Y3
C	?	-	LYS	DELETION	UNP Q8K3Y3
C	?	-	ARG	DELETION	UNP Q8K3Y3
C	?	-	ARG	DELETION	UNP Q8K3Y3
C	?	-	SER	DELETION	UNP Q8K3Y3
C	?	-	LYS	DELETION	UNP Q8K3Y3
D	?	-	LYS	DELETION	UNP Q8K3Y3
D	?	-	ASN	DELETION	UNP Q8K3Y3
D	?	-	MET	DELETION	UNP Q8K3Y3
D	?	-	GLN	DELETION	UNP Q8K3Y3
D	?	-	LYS	DELETION	UNP Q8K3Y3
D	?	-	ARG	DELETION	UNP Q8K3Y3
D	?	-	ARG	DELETION	UNP Q8K3Y3
D	?	-	SER	DELETION	UNP Q8K3Y3
D	?	-	LYS	DELETION	UNP Q8K3Y3
E	?	-	LYS	DELETION	UNP Q8K3Y3
E	?	-	ASN	DELETION	UNP Q8K3Y3
E	?	-	MET	DELETION	UNP Q8K3Y3
E	?	-	GLN	DELETION	UNP Q8K3Y3
E	?	-	LYS	DELETION	UNP Q8K3Y3
E	?	-	ARG	DELETION	UNP Q8K3Y3
E	?	-	ARG	DELETION	UNP Q8K3Y3
E	?	-	SER	DELETION	UNP Q8K3Y3
E	?	-	LYS	DELETION	UNP Q8K3Y3
F	?	-	LYS	DELETION	UNP Q8K3Y3
F	?	-	ASN	DELETION	UNP Q8K3Y3
F	?	-	MET	DELETION	UNP Q8K3Y3
F	?	-	GLN	DELETION	UNP Q8K3Y3
F	?	-	LYS	DELETION	UNP Q8K3Y3
F	?	-	ARG	DELETION	UNP Q8K3Y3
F	?	-	ARG	DELETION	UNP Q8K3Y3
F	?	-	SER	DELETION	UNP Q8K3Y3
F	?	-	LYS	DELETION	UNP Q8K3Y3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	21	Total	C	N	O	P	0	0	0
			453	202	85	146	20			
2	V	21	Total	C	N	O	P	0	0	0
			453	202	85	146	20			
2	W	21	Total	C	N	O	P	0	0	0
			453	202	85	146	20			
2	X	21	Total	C	N	O	P	0	0	0
			453	202	85	146	20			
2	Y	21	Total	C	N	O	P	0	0	0
			453	202	85	146	20			
2	Z	21	Total	C	N	O	P	0	0	0
			453	202	85	146	20			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

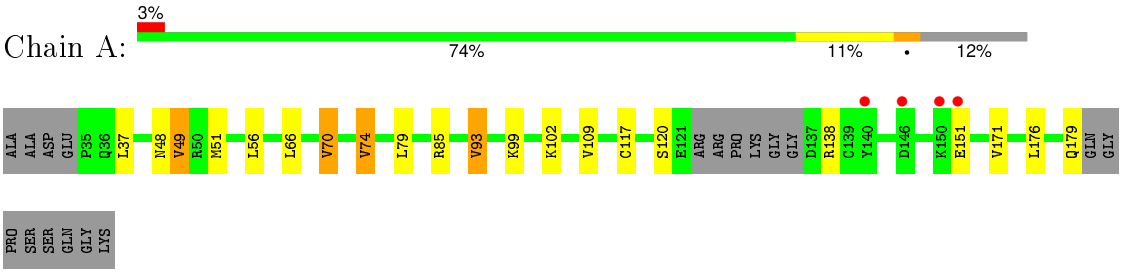
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Zn	0	0
			2	2		
3	E	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		
3	F	2	Total	Zn	0	0
			2	2		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

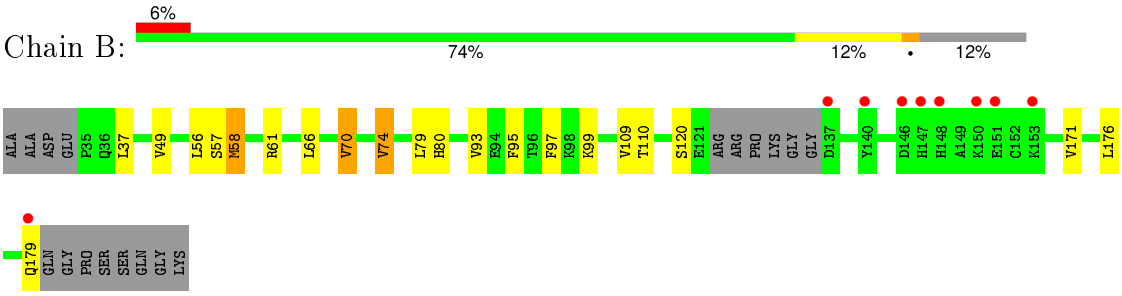
- Molecule 1: Protein lin-28 homolog A

Chain A:



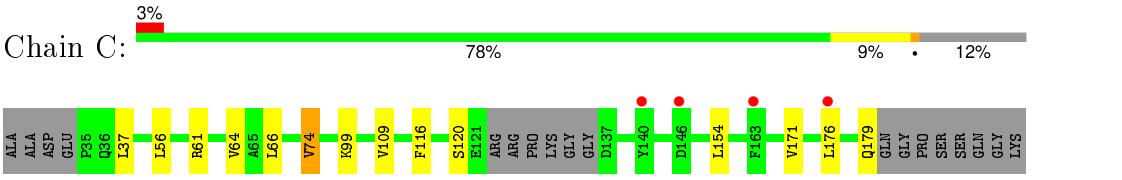
- Molecule 1: Protein lin-28 homolog A

Chain B:



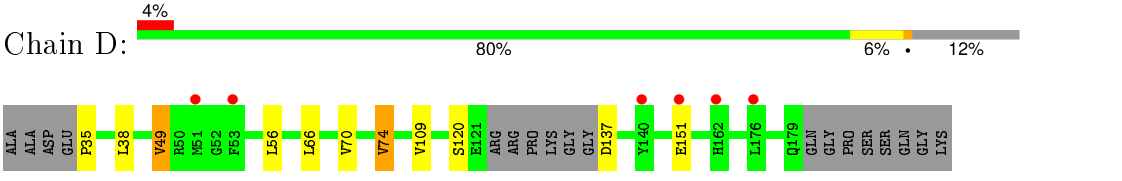
- Molecule 1: Protein lin-28 homolog A

Chain C:



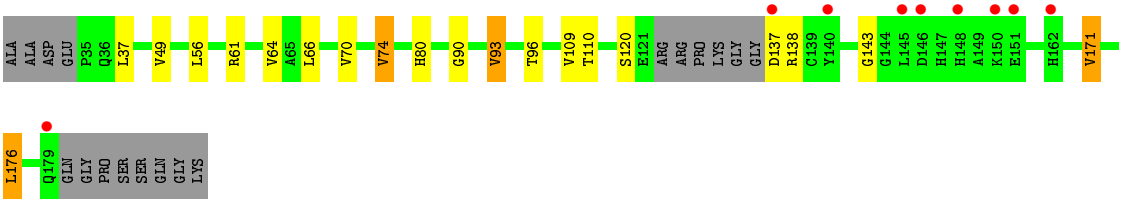
- Molecule 1: Protein lin-28 homolog A

Chain D:

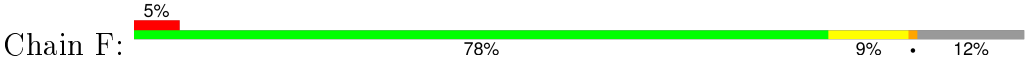


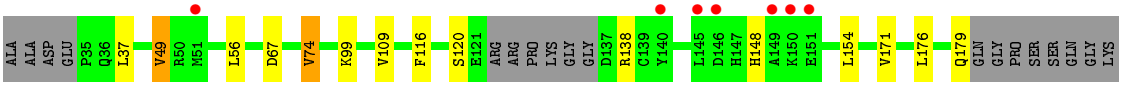
- Molecule 1: Protein lin-28 homolog A

Chain E:

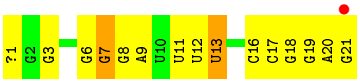


• Molecule 1: Protein lin-28 homolog A

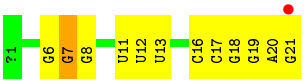




• Molecule 2: RNA (5'-R(*GP*GP*GP*CP*AP*GP*GP*GP*AP*UP*UP*UP*UP*GP*CP*CP *CP*GP*GP*AP*G)-3')

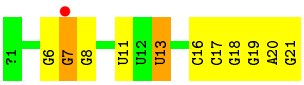


• Molecule 2: RNA (5'-R(*GP*GP*GP*CP*AP*GP*GP*GP*AP*UP*UP*UP*UP*GP*CP*CP *CP*GP*GP*AP*G)-3')



• Molecule 2: RNA (5'-R(*GP*GP*GP*CP*AP*GP*GP*GP*AP*UP*UP*UP*UP*GP*CP*CP *CP*GP*GP*AP*G)-3')

• Molecule 2: RNA (5'-R(*GP*GP*GP*CP*AP*GP*GP*GP*AP*UP*UP*UP*UP*GP*CP*CP *CP*GP*GP*AP*G)-3')

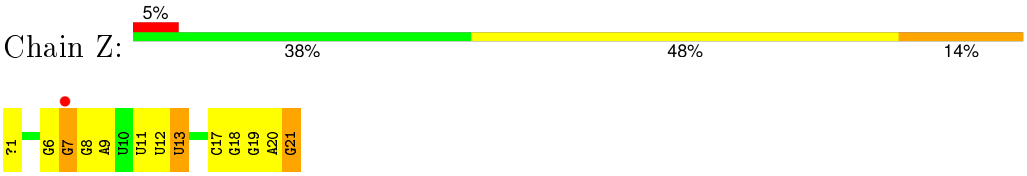


• Molecule 2: RNA (5'-R(*GP*GP*GP*CP*AP*GP*GP*GP*AP*UP*UP*UP*UP*GP*CP*CP *CP*GP*GP*AP*G)-3')

Chain Y:

• Molecule 2: RNA (5'-R(*GP*GP*GP*CP*AP*GP*GP*GP*AP*UP*UP*UP*UP*GP*CP*CP *CP*GP*GP*AP*G)-3')

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	143.82Å 143.82Å 177.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.66 – 2.90 66.66 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (66.66-2.90) 98.4 (66.66-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.183 , 0.210 0.190 , 0.216	Depositor DCC
R_{free} test set	2086 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	65.4	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	8 of 41252 reflections (0.019%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8694	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.22 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6093e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, GMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.46	0/1019	0.74	0/1366
1	B	0.47	0/1019	0.74	0/1366
1	C	0.46	0/1019	0.71	0/1366
1	D	0.48	0/1019	0.75	0/1366
1	E	0.45	0/1019	0.74	0/1366
1	F	0.45	0/1019	0.73	0/1366
2	U	0.93	0/484	1.56	9/754 (1.2%)
2	V	0.88	0/484	1.48	4/754 (0.5%)
2	W	0.92	0/484	1.50	4/754 (0.5%)
2	X	0.88	0/484	1.56	4/754 (0.5%)
2	Y	0.92	0/484	1.56	6/754 (0.8%)
2	Z	0.94	0/484	1.54	5/754 (0.7%)
All	All	0.64	0/9018	1.09	32/12720 (0.3%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	W	17	C	O4'-C1'-N1	9.04	115.43	108.20
2	U	17	C	O4'-C1'-N1	8.59	115.07	108.20
2	Y	17	C	O4'-C1'-N1	8.19	114.75	108.20
2	Z	17	C	O4'-C1'-N1	8.02	114.61	108.20
2	X	17	C	O4'-C1'-N1	7.90	114.52	108.20
2	V	17	C	O4'-C1'-N1	7.70	114.36	108.20
2	Z	7	G	C1'-O4'-C4'	-6.97	104.32	109.90
2	X	7	G	C1'-O4'-C4'	-6.86	104.41	109.90
2	V	7	G	C1'-O4'-C4'	-6.66	104.57	109.90
2	Y	7	G	C1'-O4'-C4'	-6.60	104.62	109.90
2	W	7	G	C1'-O4'-C4'	-6.47	104.72	109.90
2	U	7	G	C1'-O4'-C4'	-6.32	104.85	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	U	7	G	P-O3'-C3'	5.81	126.68	119.70
2	Y	7	G	P-O3'-C3'	5.80	126.66	119.70
2	Z	12	U	P-O3'-C3'	5.75	126.60	119.70
2	X	16	C	O4'-C1'-N1	5.75	112.80	108.20
2	U	9	A	P-O3'-C3'	5.52	126.33	119.70
2	W	7	G	P-O3'-C3'	5.51	126.32	119.70
2	U	12	U	P-O3'-C3'	5.48	126.28	119.70
2	V	12	U	P-O3'-C3'	5.47	126.26	119.70
2	Z	7	G	P-O3'-C3'	5.46	126.26	119.70
2	X	7	G	P-O3'-C3'	5.41	126.19	119.70
2	V	16	C	O4'-C1'-N1	5.40	112.52	108.20
2	U	16	C	O4'-C1'-N1	5.37	112.49	108.20
2	W	16	C	O4'-C1'-N1	5.34	112.47	108.20
2	Z	9	A	P-O3'-C3'	5.27	126.02	119.70
2	U	3	G	O4'-C1'-N9	5.21	112.37	108.20
2	U	9	A	N1-C6-N6	5.12	121.67	118.60
2	Y	12	U	P-O3'-C3'	5.10	125.82	119.70
2	Y	21	G	C8-N9-C4	-5.09	104.36	106.40
2	Y	16	C	O4'-C1'-N1	5.02	112.22	108.20
2	U	9	A	C5-C6-N6	-5.02	119.68	123.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	994	0	981	8	0
1	B	994	0	981	10	0
1	C	994	0	981	5	0
1	D	994	0	981	5	0
1	E	994	0	981	10	0
1	F	994	0	981	6	0
2	U	453	0	229	2	0
2	V	453	0	229	0	0
2	W	453	0	229	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	453	0	229	1	0
2	Y	453	0	229	1	0
2	Z	453	0	229	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
All	All	8694	0	7260	42	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 3.

All (42) 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:D:66:LEU:HD13	1:D:70:VAL:HG13	1.82	0.60
1:B:66:LEU:HD13	1:B:70:VAL:HG13	1.83	0.60
1:C:61:ARG:HB2	1:C:66:LEU:HD11	1.90	0.54
1:B:58:MET:HG3	1:B:95:PHE:HZ	1.72	0.54
1:C:56:LEU:HG	1:C:74:VAL:HG22	1.90	0.54
1:D:56:LEU:HG	1:D:74:VAL:HG22	1.89	0.53
1:A:117:CYS:O	1:A:138:ARG:NH2	2.41	0.52
1:E:56:LEU:HD22	1:E:93:VAL:HG11	1.93	0.51
1:A:48:ASN:HB3	1:A:51:MET:HB2	1.92	0.50
1:E:56:LEU:HG	1:E:74:VAL:HG22	1.95	0.48
1:A:66:LEU:HD13	1:A:70:VAL:HG13	1.96	0.47
1:E:90:GLY:HA3	1:E:176:LEU:HD21	1.97	0.46
1:D:74:VAL:CG1	1:D:109:VAL:HG21	2.46	0.46
1:B:74:VAL:CG1	1:B:109:VAL:HG21	2.46	0.46
1:B:56:LEU:HD22	1:B:93:VAL:HG21	1.97	0.45
1:A:49:VAL:HG22	2:U:13:U:C2	2.52	0.45
1:E:74:VAL:CG1	1:E:109:VAL:HG21	2.47	0.45
1:A:74:VAL:CG1	1:A:109:VAL:HG21	2.47	0.45
1:F:74:VAL:CG1	1:F:109:VAL:HG21	2.48	0.44
1:C:74:VAL:CG1	1:C:109:VAL:HG21	2.48	0.44
1:A:56:LEU:HD22	1:A:93:VAL:HG11	1.99	0.44
1:F:56:LEU:HG	1:F:74:VAL:HG22	1.98	0.44
1:F:148:HIS:CE1	2:Y:21:G:H2'	2.53	0.44
1:E:138:ARG:HE	1:E:143:GLY:HA2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LEU:HD21	1:F:116:PHE:HE1	1.83	0.43
1:B:58:MET:HG3	1:B:95:PHE:CZ	2.52	0.43
1:E:80:HIS:HB3	1:E:110:THR:HG22	2.01	0.43
1:F:49:VAL:HG22	2:Z:13:U:C2	2.54	0.43
1:C:116:PHE:HE1	1:F:154:LEU:HD21	1.83	0.43
1:E:61:ARG:HB2	1:E:66:LEU:HD11	2.01	0.42
1:B:171:VAL:HG21	2:U:1:GMP:C6	2.55	0.42
1:E:80:HIS:CB	1:E:110:THR:HG22	2.49	0.42
1:D:49:VAL:HG22	2:X:13:U:C2	2.54	0.42
1:B:79:LEU:HD23	1:B:109:VAL:HB	2.02	0.42
1:B:58:MET:HE1	1:B:97:PHE:CZ	2.54	0.41
1:D:35:PRO:HB2	1:D:38:LEU:HD21	2.02	0.41
1:B:61:ARG:HB2	1:B:66:LEU:HD11	2.01	0.41
1:E:137:ASP:HB2	2:Z:21:G:N2	2.36	0.41
1:E:171:VAL:HG21	2:Z:1:GMP:C6	2.57	0.40
1:B:80:HIS:CB	1:B:110:THR:HG22	2.51	0.40
1:A:56:LEU:HG	1:A:74:VAL:HG22	2.03	0.40
1:A:79:LEU:HD12	1:A:85:ARG:HB3	2.02	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
1	A	126/148 (85%)	123 (98%)	2 (2%)	1 (1%)	24 60
1	B	126/148 (85%)	123 (98%)	3 (2%)	0	100 100
1	C	126/148 (85%)	123 (98%)	2 (2%)	1 (1%)	24 60
1	D	126/148 (85%)	122 (97%)	4 (3%)	0	100 100
1	E	126/148 (85%)	124 (98%)	1 (1%)	1 (1%)	24 60
1	F	126/148 (85%)	123 (98%)	2 (2%)	1 (1%)	24 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	756/888 (85%)	738 (98%)	14 (2%)	4 (0%)	34 71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	VAL
1	F	171	VAL
1	E	171	VAL
1	C	171	VAL

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	107/119 (90%)	96 (90%)	11 (10%)	9 26
1	B	107/119 (90%)	97 (91%)	10 (9%)	11 32
1	C	107/119 (90%)	100 (94%)	7 (6%)	21 52
1	D	107/119 (90%)	102 (95%)	5 (5%)	32 68
1	E	107/119 (90%)	98 (92%)	9 (8%)	14 37
1	F	107/119 (90%)	98 (92%)	9 (8%)	14 37
All	All	642/714 (90%)	591 (92%)	51 (8%)	15 41

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	49	VAL
1	A	70	VAL
1	A	74	VAL
1	A	93	VAL
1	A	99	LYS
1	A	102	LYS
1	A	120	SER

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Mol	Chain	Res	Type
1	A	151	GLU
1	A	176	LEU
1	A	179	GLN
1	B	37	LEU
1	B	49	VAL
1	B	57	SER
1	B	58	MET
1	B	70	VAL
1	B	74	VAL
1	B	99	LYS
1	B	120	SER
1	B	176	LEU
1	B	179	GLN
1	C	37	LEU
1	C	64	VAL
1	C	74	VAL
1	C	99	LYS
1	C	120	SER
1	C	176	LEU
1	C	179	GLN
1	D	49	VAL
1	D	74	VAL
1	D	120	SER
1	D	137	ASP
1	D	151	GLU
1	E	37	LEU
1	E	49	VAL
1	E	64	VAL
1	E	70	VAL
1	E	74	VAL
1	E	93	VAL
1	E	96	THR
1	E	120	SER
1	E	176	LEU
1	F	37	LEU
1	F	49	VAL
1	F	67	ASP
1	F	74	VAL
1	F	99	LYS
1	F	120	SER
1	F	138	ARG
1	F	176	LEU

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Mol	Chain	Res	Type
1	F	179	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	39	HIS
1	C	165	GLN
1	D	39	HIS
1	D	148	HIS
1	D	165	GLN
1	E	165	GLN
1	F	148	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	U	19/21 (90%)	7 (36%)	3 (15%)
2	V	19/21 (90%)	7 (36%)	3 (15%)
2	W	19/21 (90%)	7 (36%)	3 (15%)
2	X	19/21 (90%)	7 (36%)	3 (15%)
2	Y	19/21 (90%)	7 (36%)	3 (15%)
2	Z	19/21 (90%)	7 (36%)	3 (15%)
All	All	114/126 (90%)	42 (36%)	18 (15%)

All (42) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	U	6	G
2	U	7	G
2	U	8	G
2	U	13	U
2	U	18	G
2	U	20	A
2	U	21	G
2	V	6	G
2	V	7	G
2	V	8	G
2	V	13	U
2	V	18	G
2	V	20	A

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Mol	Chain	Res	Type
2	V	21	G
2	W	6	G
2	W	7	G
2	W	8	G
2	W	13	U
2	W	18	G
2	W	20	A
2	W	21	G
2	X	6	G
2	X	7	G
2	X	8	G
2	X	13	U
2	X	18	G
2	X	20	A
2	X	21	G
2	Y	6	G
2	Y	7	G
2	Y	8	G
2	Y	13	U
2	Y	18	G
2	Y	20	A
2	Y	21	G
2	Z	6	G
2	Z	7	G
2	Z	8	G
2	Z	13	U
2	Z	18	G
2	Z	20	A
2	Z	21	G

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	U	7	G
2	U	11	U
2	U	19	G
2	V	7	G
2	V	11	U
2	V	19	G
2	W	7	G
2	W	11	U
2	W	19	G

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Mol	Chain	Res	Type
2	X	7	G
2	X	11	U
2	X	19	G
2	Y	7	G
2	Y	11	U
2	Y	19	G
2	Z	7	G
2	Z	11	U
2	Z	19	G

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 95^{th} 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	A	130/148 (87%)	0.55	4 (3%) 52 45	39, 56, 91, 117	0
1	B	130/148 (87%)	0.54	9 (6%) 20 14	39, 59, 95, 120	0
1	C	130/148 (87%)	0.56	4 (3%) 52 45	43, 61, 97, 130	0
1	D	130/148 (87%)	0.50	6 (4%) 36 30	42, 60, 93, 120	0
1	E	130/148 (87%)	0.61	9 (6%) 20 14	45, 61, 97, 140	0
1	F	130/148 (87%)	0.50	7 (5%) 29 23	46, 63, 98, 119	0
2	U	20/21 (95%)	0.39	1 (5%) 32 26	52, 78, 118, 121	0
2	V	20/21 (95%)	0.37	1 (5%) 32 26	65, 83, 114, 116	0
2	W	20/21 (95%)	0.40	1 (5%) 32 26	60, 82, 124, 124	0
2	X	20/21 (95%)	0.34	1 (5%) 32 26	74, 85, 116, 116	0
2	Y	20/21 (95%)	0.38	0 100 100	58, 84, 121, 125	0
2	Z	20/21 (95%)	0.46	1 (5%) 32 26	80, 88, 120, 120	0
All	All	900/1014 (88%)	0.53	44 (4%) 33 27	39, 63, 101, 140	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	GLU	5.1
1	D	151	GLU	3.8
1	C	140	TYR	3.6
1	D	140	TYR	3.5
1	D	51	MET	3.3
1	E	179	GLN	3.3
1	E	150	LYS	3.1
1	F	150	LYS	3.0
1	A	151	GLU	2.9
1	E	137	ASP	2.8
1	E	151	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	140	TYR	2.8
1	B	150	LYS	2.8
1	B	179	GLN	2.8
1	B	146	ASP	2.8
1	E	146	ASP	2.8
1	E	140	TYR	2.8
1	A	150	LYS	2.7
1	F	51	MET	2.7
1	B	148	HIS	2.7
1	F	146	ASP	2.7
1	C	176	LEU	2.6
1	C	146	ASP	2.6
1	E	162	HIS	2.6
1	D	162	HIS	2.5
1	F	149	ALA	2.5
1	F	145	LEU	2.4
1	B	140	TYR	2.4
1	F	140	TYR	2.4
2	X	7	G	2.4
1	D	176	LEU	2.3
1	F	151	GLU	2.3
1	C	163	PHE	2.3
1	E	145	LEU	2.2
1	E	148	HIS	2.2
2	W	21	G	2.2
1	D	53	PHE	2.2
1	B	137	ASP	2.1
1	B	153	LYS	2.1
1	A	146	ASP	2.1
1	B	147	HIS	2.1
2	V	21	G	2.1
2	Z	7	G	2.1
2	U	21	G	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 carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	A	2	1/1	1.00	0.18	-0.37	52,52,52,52	0
3	ZN	F	2	1/1	1.00	0.19	-0.49	57,57,57,57	0
3	ZN	D	2	1/1	1.00	0.17	-0.76	54,54,54,54	0
3	ZN	B	2	1/1	1.00	0.18	-0.81	52,52,52,52	0
3	ZN	C	2	1/1	1.00	0.14	-0.90	64,64,64,64	0
3	ZN	A	1	1/1	1.00	0.15	-1.07	71,71,71,71	0
3	ZN	E	2	1/1	1.00	0.11	-1.26	64,64,64,64	0
3	ZN	E	1	1/1	0.99	0.14	-1.39	71,71,71,71	0
3	ZN	C	1	1/1	1.00	0.14	-1.49	71,71,71,71	0
3	ZN	F	1	1/1	0.99	0.13	-1.71	69,69,69,69	0
3	ZN	B	1	1/1	1.00	0.14	-1.76	69,69,69,69	0
3	ZN	D	1	1/1	0.99	0.14	-2.15	69,69,69,69	0

6.5 Other polymers

There are no such residues in this entry.