



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:19 PM GMT

PDB ID : 4L8R  
Title : Structure of mrna stem-loop, human stem-loop binding protein and 3'hexo  
ternary complex  
Authors : Tan, D.; Tong, L.  
Deposited on : 2013-06-17  
Resolution : 2.60 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

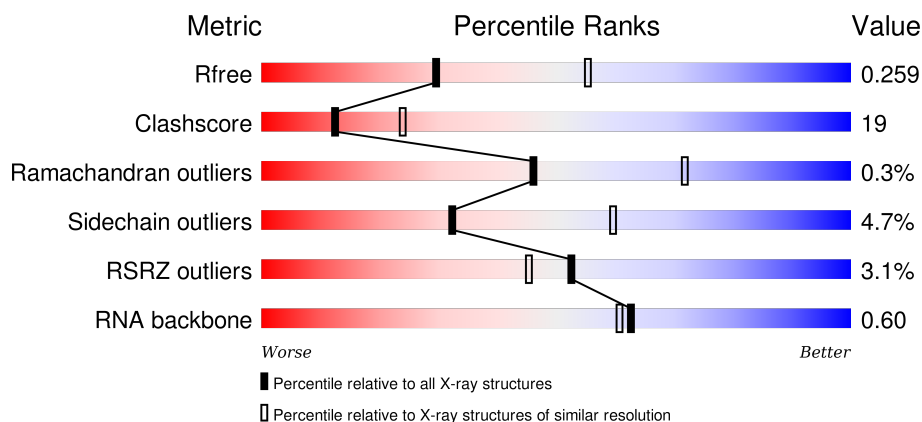
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)
RNA backbone	2183	1022 (3.00-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	26	
1	D	26	
2	B	303	
2	E	303	

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Mol	Chain	Length	Quality of chain
3	C	120	<p>6% 26% 29% 44%</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6136 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 HISTONE MRNA STEM-LOOP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	26	Total	C	N	O	P	0	0	0
			543	245	95	178	25			
1	D	19	Total	C	N	O	P	0	0	1
			375	168	61	128	18			

- Molecule 2 is a protein called 3'-5' exoribonuclease 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	276	Total	C	N	O	S	Se	0	0	0
			2257	1444	379	417	7	10			
2	E	274	Total	C	N	O	S	Se	0	0	0
			2242	1438	377	410	7	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	350	LEU	-	EXPRESSION TAG	UNP Q8IV48
B	351	GLU	-	EXPRESSION TAG	UNP Q8IV48
B	352	HIS	-	EXPRESSION TAG	UNP Q8IV48
B	353	HIS	-	EXPRESSION TAG	UNP Q8IV48
B	354	HIS	-	EXPRESSION TAG	UNP Q8IV48
B	355	HIS	-	EXPRESSION TAG	UNP Q8IV48
B	356	HIS	-	EXPRESSION TAG	UNP Q8IV48
B	357	HIS	-	EXPRESSION TAG	UNP Q8IV48
E	350	LEU	-	EXPRESSION TAG	UNP Q8IV48
E	351	GLU	-	EXPRESSION TAG	UNP Q8IV48
E	352	HIS	-	EXPRESSION TAG	UNP Q8IV48
E	353	HIS	-	EXPRESSION TAG	UNP Q8IV48
E	354	HIS	-	EXPRESSION TAG	UNP Q8IV48
E	355	HIS	-	EXPRESSION TAG	UNP Q8IV48
E	356	HIS	-	EXPRESSION TAG	UNP Q8IV48
E	357	HIS	-	EXPRESSION TAG	UNP Q8IV48

- Molecule 3 is a protein called Histone RNA hairpin-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	67	Total	C	N	O	S	0	0	0
			584	378	105	100	1			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	104	MET	-	EXPRESSION TAG	UNP Q14493
C	105	GLY	-	EXPRESSION TAG	UNP Q14493
C	106	SER	-	EXPRESSION TAG	UNP Q14493
C	107	SER	-	EXPRESSION TAG	UNP Q14493
C	108	HIS	-	EXPRESSION TAG	UNP Q14493
C	109	HIS	-	EXPRESSION TAG	UNP Q14493
C	110	HIS	-	EXPRESSION TAG	UNP Q14493
C	111	HIS	-	EXPRESSION TAG	UNP Q14493
C	112	HIS	-	EXPRESSION TAG	UNP Q14493
C	113	HIS	-	EXPRESSION TAG	UNP Q14493
C	114	SER	-	EXPRESSION TAG	UNP Q14493
C	115	SER	-	EXPRESSION TAG	UNP Q14493
C	116	GLY	-	EXPRESSION TAG	UNP Q14493
C	117	LEU	-	EXPRESSION TAG	UNP Q14493
C	118	VAL	-	EXPRESSION TAG	UNP Q14493
C	119	PRO	-	EXPRESSION TAG	UNP Q14493
C	120	ARG	-	EXPRESSION TAG	UNP Q14493
C	121	GLY	-	EXPRESSION TAG	UNP Q14493
C	122	SER	-	EXPRESSION TAG	UNP Q14493
C	123	HIS	-	EXPRESSION TAG	UNP Q14493
C	124	MET	-	EXPRESSION TAG	UNP Q14493

- Molecule 4 is water.

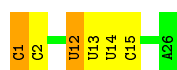
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	52	Total	O	0	0
			52	52		
4	C	14	Total	O	0	0
			14	14		
4	D	9	Total	O	0	0
			9	9		
4	E	42	Total	O	0	0
			42	42		

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


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: HISTONE MRNA STEM-LOOP

Chain A: 



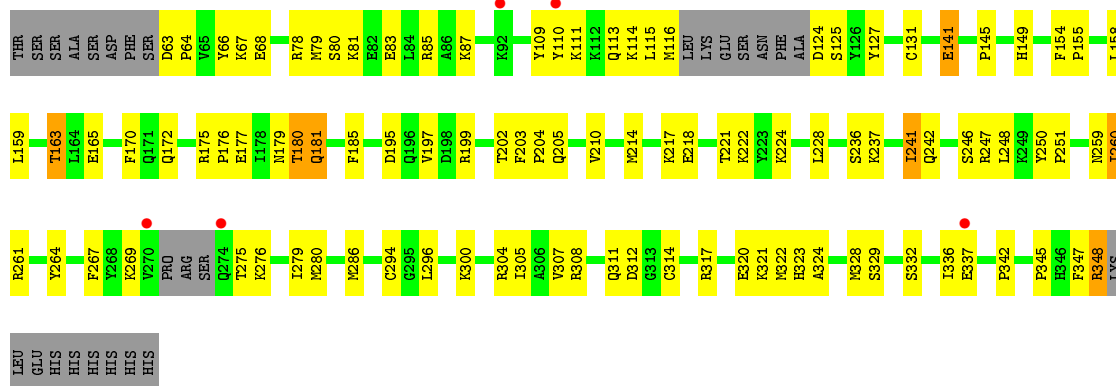
#### • Molecule 1: HISTONE MRNA STEM-LOOP

Chain D: 



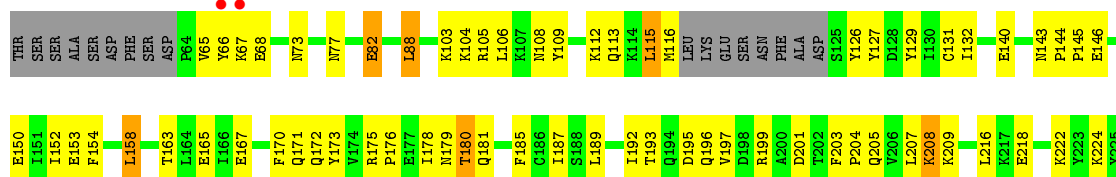
#### • Molecule 2: 3'-5' exoribonuclease 1

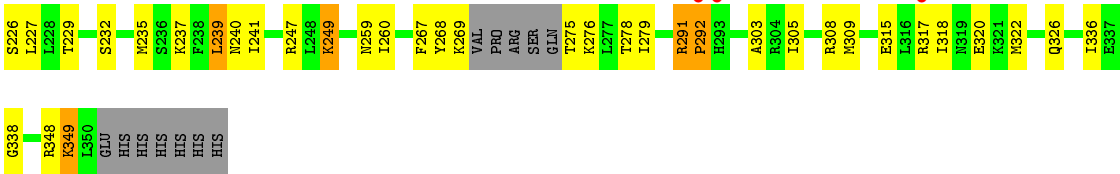
Chain B: 



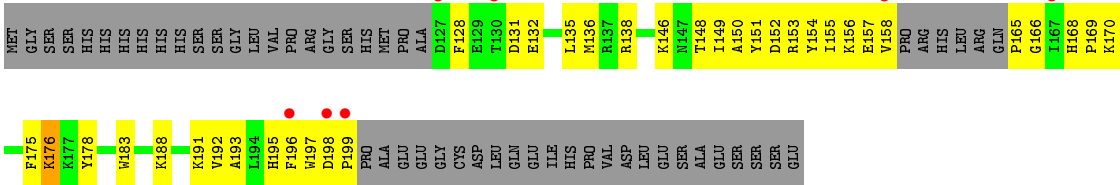
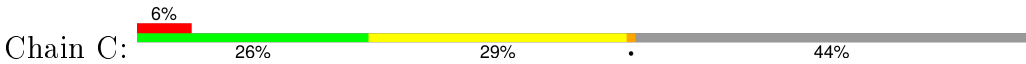
#### • Molecule 2: 3'-5' exoribonuclease 1

Chain E: 





● Molecule 3: Histone RNA hairpin-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.76 Å 90.80 Å 128.64 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.93 – 2.60 37.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.0 (37.93-2.60) 97.3 (37.93-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.61 Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.199 , 0.249 0.211 , 0.259	Depositor DCC
$R_{free}$ test set	1453 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.813	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 55841 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.54	1/605 (0.2%)	0.80	2/939 (0.2%)
1	D	0.54	1/416 (0.2%)	0.68	0/645
2	B	0.50	0/2293	0.67	1/3070 (0.0%)
2	E	0.49	0/2278	0.66	0/3047
3	C	0.61	2/601 (0.3%)	0.62	0/807
All	All	0.51	4/6193 (0.1%)	0.68	3/8508 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	8	C	O3'-P	-10.56	1.48	1.61
1	A	1	C	O3'-P	-8.89	1.50	1.61
3	C	157	GLU	CD-OE1	-5.71	1.19	1.25
3	C	157	GLU	C-O	-5.39	1.13	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	294	CYS	N-CA-C	-6.30	93.99	111.00
1	A	1	C	C3'-C2'-O2'	5.50	129.26	113.30
1	A	1	C	C1'-C2'-O2'	-5.02	95.54	110.60

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	543	0	283	10	0
1	D	375	0	194	6	0
2	B	2257	0	2281	90	0
2	E	2242	0	2281	96	0
3	C	584	0	580	33	0
4	A	18	0	0	1	0
4	B	52	0	0	6	0
4	C	14	0	0	0	0
4	D	9	0	0	1	0
4	E	42	0	0	2	0
All	All	6136	0	5619	226	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 19.

All (226) 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:B:236:SER:HA	2:B:322:MSE:HE1	1.31	1.07
2:E:349:LYS:HD3	2:E:349:LYS:H	1.40	0.87
2:B:348:ARG:HB2	2:B:348:ARG:NH1	1.88	0.87
2:E:224:LYS:HE3	2:E:338:GLY:HA3	1.55	0.87
2:B:115:LEU:O	2:B:116:MSE:HG3	1.75	0.86
2:E:249:LYS:HD3	2:E:348:ARG:HD2	1.57	0.86
2:B:80:SER:OG	2:B:83:GLU:HG3	1.78	0.83
2:B:149:HIS:O	2:B:241:ILE:HD11	1.78	0.83
3:C:165:PRO:HB3	3:C:168:HIS:CD2	2.14	0.82
1:A:1:C:C5'	1:A:1:C:O2	2.27	0.82
2:B:81:LYS:HE2	2:B:85:ARG:NH2	1.98	0.79
2:B:280:MSE:HE2	2:B:305:ILE:HG21	1.63	0.79
2:E:237:LYS:O	2:E:241:ILE:HG12	1.83	0.78
2:E:349:LYS:HD3	2:E:349:LYS:N	1.99	0.76
2:B:264:TYR:CD2	2:B:280:MSE:HE3	2.22	0.75
2:E:308:ARG:HD3	2:E:308:ARG:O	1.87	0.75
2:E:170:PHE:CZ	2:E:172:GLN:HG3	2.23	0.74
2:B:68:GLU:OE2	2:B:114:LYS:HD3	1.88	0.73
2:B:308:ARG:O	2:B:308:ARG:HD3	1.88	0.72
2:E:349:LYS:H	2:E:349:LYS:CD	1.94	0.72
2:B:81:LYS:HE2	2:B:85:ARG:HH21	1.54	0.72
2:E:129:TYR:HE2	2:E:167:GLU:HG3	1.53	0.72
2:E:260:ILE:HG13	2:E:309:MSE:HE1	1.72	0.70
2:E:226:SER:OG	2:E:318:ILE:HD11	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:SER:CA	2:B:322:MSE:HE1	2.16	0.69
3:C:150:ALA:HB2	3:C:198:ASP:OD2	1.92	0.69
1:A:1:C:H5"	1:A:1:C:O2	1.92	0.69
3:C:176:LYS:HB3	3:C:178:TYR:CE2	2.27	0.68
2:E:260:ILE:CG1	2:E:309:MSE:HE1	2.23	0.68
3:C:165:PRO:HB3	3:C:168:HIS:HD2	1.58	0.68
2:E:109:TYR:O	2:E:113:GLN:HG2	1.93	0.68
3:C:198:ASP:HB3	3:C:199:PRO:CD	2.24	0.68
2:E:193:THR:HG23	4:E:413:HOH:O	1.93	0.68
2:B:286:MSE:HE1	2:B:304:ARG:HB3	1.77	0.67
1:D:14:U:OP2	2:E:67:LYS:NZ	2.26	0.67
3:C:148:THR:HG22	3:C:150:ALA:H	1.60	0.67
2:B:348:ARG:CZ	2:B:348:ARG:HB2	2.26	0.66
3:C:158:VAL:HG11	3:C:168:HIS:CD2	2.31	0.66
3:C:154:TYR:OH	3:C:168:HIS:HB3	1.97	0.65
2:B:79:MSE:HE1	2:B:87:LYS:HG3	1.79	0.65
2:E:249:LYS:HD2	2:E:349:LYS:HZ3	1.60	0.65
2:E:260:ILE:HD11	2:E:309:MSE:CE	2.27	0.65
2:E:247:ARG:NH1	2:E:348:ARG:O	2.29	0.64
3:C:196:PHE:HB3	3:C:197:TRP:CZ3	2.32	0.64
3:C:149:ILE:O	3:C:153:ARG:HG2	1.97	0.64
2:E:178:ILE:HG13	2:E:179:ASN:N	2.11	0.64
3:C:198:ASP:HB3	3:C:199:PRO:HD2	1.81	0.63
3:C:152:ASP:O	3:C:156:LYS:HG3	1.99	0.63
2:E:180:THR:HG22	2:E:181:GLN:HG2	1.81	0.63
2:E:232:SER:HB3	2:E:320:GLU:OE1	2.00	0.61
2:B:260:ILE:HG23	2:B:280:MSE:HE1	1.83	0.60
3:C:132:GLU:HG3	3:C:136:MET:CE	2.30	0.60
2:E:218:GLU:OE2	2:E:222:LYS:HD3	2.01	0.60
2:E:195:ASP:O	2:E:199:ARG:HG2	2.02	0.60
1:A:15:C:H42	3:C:199:PRO:HD2	1.66	0.59
2:B:109:TYR:O	2:B:113:GLN:HG2	2.01	0.59
1:A:15:C:O2	2:B:78:ARG:NH2	2.35	0.59
2:B:87:LYS:HE2	2:B:87:LYS:HA	1.83	0.59
3:C:196:PHE:HB3	3:C:197:TRP:CE3	2.38	0.58
2:E:193:THR:HG22	2:E:196:GLN:H	1.69	0.58
2:E:143:ASN:N	2:E:144:PRO:HD3	2.17	0.58
2:B:180:THR:HG22	2:B:181:GLN:OE1	2.04	0.58
3:C:158:VAL:HG21	3:C:168:HIS:CE1	2.39	0.58
2:B:264:TYR:CG	2:B:280:MSE:HE3	2.38	0.57
2:E:276:LYS:HZ3	2:E:278:THR:H	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:260:ILE:HD11	2:E:309:MSE:HE2	1.85	0.57
3:C:195:HIS:C	3:C:197:TRP:H	2.08	0.57
2:E:276:LYS:HG2	2:E:279:ILE:HG12	1.87	0.57
2:B:323:HIS:O	2:B:324:ALA:HB3	2.04	0.57
2:E:126:TYR:CD2	2:E:336:ILE:HG22	2.40	0.56
2:E:77:ASN:OD1	2:E:103:LYS:HE3	2.05	0.56
2:E:176:PRO:HD3	2:E:197:VAL:CG1	2.36	0.56
1:A:1:C:C4'	1:A:1:C:O2	2.54	0.56
2:E:276:LYS:HZ2	2:E:278:THR:HB	1.70	0.55
2:B:348:ARG:HB2	2:B:348:ARG:HH11	1.69	0.55
2:B:264:TYR:HB2	2:B:280:MSE:HE3	1.87	0.55
2:E:152:ILE:HG22	2:E:176:PRO:HG3	1.89	0.55
2:B:236:SER:HA	2:B:322:MSE:CE	2.22	0.55
3:C:132:GLU:HG3	3:C:136:MET:HE1	1.89	0.55
2:E:150:GLU:OE2	2:E:179:ASN:HB2	2.07	0.54
2:B:321:LYS:HE2	2:B:328:MSE:HE2	1.88	0.54
2:B:110:TYR:O	2:B:111:LYS:C	2.44	0.54
2:B:170:PHE:CE1	2:B:210:VAL:HG22	2.42	0.54
2:E:276:LYS:CD	2:E:278:THR:HG22	2.38	0.54
3:C:195:HIS:C	3:C:197:TRP:N	2.59	0.54
2:E:127:TYR:OH	2:E:318:ILE:HD13	2.09	0.53
2:B:124:ASP:OD2	2:B:125:SER:N	2.34	0.53
2:B:179:ASN:HA	4:B:439:HOH:O	2.07	0.53
2:E:201:ASP:OD2	2:E:209:LYS:NZ	2.39	0.53
2:B:141:GLU:HG2	2:B:185:PHE:CD2	2.44	0.53
2:B:145:PRO:HD3	2:E:326:GLN:HG2	1.91	0.53
2:B:195:ASP:O	2:B:199:ARG:HG2	2.09	0.53
2:E:276:LYS:CG	2:E:279:ILE:HG12	2.39	0.53
2:E:176:PRO:HD3	2:E:197:VAL:HG13	1.91	0.52
2:E:175:ARG:HA	2:E:197:VAL:HG13	1.91	0.52
2:B:163:THR:HG22	2:B:165:GLU:N	2.24	0.52
2:B:236:SER:O	2:E:146:GLU:HG3	2.09	0.52
2:E:82:GLU:H	2:E:82:GLU:CD	2.12	0.52
2:E:315:GLU:O	2:E:317:ARG:NH1	2.32	0.52
2:B:251:PRO:HG3	2:B:345:PRO:HG3	1.91	0.52
2:E:276:LYS:NZ	2:E:278:THR:HB	2.25	0.52
2:E:140:GLU:OE2	2:E:140:GLU:HA	2.10	0.52
2:E:260:ILE:HD11	2:E:309:MSE:HE1	1.92	0.52
2:B:195:ASP:OD2	2:B:199:ARG:NH1	2.42	0.52
2:B:64:PRO:O	2:B:67:LYS:HB2	2.09	0.52
3:C:188:LYS:O	3:C:192:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:SER:HB2	4:B:448:HOH:O	2.09	0.52
2:E:260:ILE:CD1	2:E:309:MSE:HE1	2.40	0.51
2:B:317:ARG:NH1	2:B:332:SER:O	2.43	0.51
2:B:163:THR:HG22	2:B:165:GLU:H	1.75	0.51
2:B:347:PHE:O	2:B:348:ARG:CB	2.59	0.51
3:C:152:ASP:HA	3:C:155:ILE:HG12	1.92	0.50
2:E:276:LYS:NZ	2:E:278:THR:HG22	2.27	0.50
2:E:240:ASN:ND2	2:E:322:MSE:HE1	2.27	0.50
2:B:241:ILE:HG13	2:B:242:GLN:N	2.25	0.50
2:E:104:LYS:HE3	2:E:267:PHE:O	2.12	0.50
2:E:291:ARG:HH11	2:E:291:ARG:HG3	1.77	0.50
2:E:178:ILE:CG1	2:E:179:ASN:N	2.74	0.49
2:E:185:PHE:CE1	2:E:189:LEU:HD22	2.46	0.49
1:A:1:C:H2'	1:A:2:C:H5'	1.93	0.49
2:E:115:LEU:O	2:E:116:MSE:HG2	2.12	0.49
2:B:141:GLU:HB2	4:B:428:HOH:O	2.11	0.49
2:E:249:LYS:HD2	2:E:349:LYS:NZ	2.28	0.49
2:E:126:TYR:OH	2:E:224:LYS:HE2	2.13	0.49
2:B:307:VAL:O	2:B:311:GLN:HG3	2.13	0.49
2:B:170:PHE:CZ	2:B:172:GLN:HG3	2.47	0.49
2:B:269:LYS:HE3	4:B:421:HOH:O	2.12	0.49
2:B:276:LYS:HB2	2:B:279:ILE:HG12	1.95	0.49
2:E:150:GLU:CD	2:E:178:ILE:HG12	2.33	0.49
2:B:267:PHE:CE1	2:B:314:CYS:HB2	2.48	0.48
2:E:65:VAL:HG12	2:E:68:GLU:OE1	2.13	0.48
1:A:1:C:O4'	1:A:1:C:O2	2.29	0.48
3:C:197:TRP:O	3:C:198:ASP:OD1	2.31	0.48
2:E:315:GLU:O	2:E:317:ARG:HD3	2.14	0.48
2:B:127:TYR:HE1	2:B:337:GLU:O	1.97	0.48
2:B:348:ARG:CB	2:B:348:ARG:NH1	2.71	0.47
3:C:132:GLU:HG3	3:C:136:MET:HE2	1.96	0.47
2:B:176:PRO:HD2	2:B:197:VAL:CG1	2.45	0.47
2:E:308:ARG:HD3	2:E:308:ARG:C	2.33	0.47
3:C:128:PHE:HB3	3:C:175:PHE:O	2.14	0.47
1:D:19:G:OP1	2:E:317:ARG:NH2	2.47	0.47
2:B:264:TYR:CB	2:B:280:MSE:HE3	2.44	0.47
2:B:296:LEU:HG	2:B:300:LYS:HE3	1.97	0.47
2:B:177:GLU:OE2	2:B:202:THR:HG22	2.15	0.47
2:E:205:GLN:HB3	4:E:440:HOH:O	2.15	0.47
2:E:276:LYS:HZ3	2:E:278:THR:HG22	1.80	0.47
2:E:249:LYS:CD	2:E:349:LYS:HZ3	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:LYS:HB2	2:B:224:LYS:HE3	1.72	0.46
2:E:259:ASN:HB2	2:E:320:GLU:OE1	2.15	0.46
2:B:176:PRO:HD2	2:B:197:VAL:HG13	1.98	0.46
2:E:239:LEU:O	2:E:239:LEU:HD22	2.16	0.46
2:B:347:PHE:O	2:B:348:ARG:HB3	2.16	0.46
2:B:246:SER:O	2:B:247:ARG:HB2	2.14	0.46
2:E:203:PHE:HB3	2:E:204:PRO:HD3	1.98	0.46
2:E:193:THR:HB	2:E:196:GLN:HG3	1.98	0.46
2:E:291:ARG:HD3	2:E:291:ARG:O	2.16	0.46
1:A:13:U:O4'	2:B:66:TYR:HB3	2.15	0.46
2:E:276:LYS:HD3	2:E:278:THR:HG22	1.96	0.46
2:B:163:THR:CG2	2:B:165:GLU:HB2	2.46	0.45
2:B:110:TYR:O	2:B:113:GLN:N	2.49	0.45
2:E:276:LYS:HG3	2:E:278:THR:HG22	1.98	0.45
2:E:187:ILE:HG23	2:E:192:ILE:O	2.16	0.45
1:D:13:U:O4'	2:E:66:TYR:HB3	2.16	0.45
2:B:348:ARG:HH11	2:B:348:ARG:CB	2.28	0.45
2:B:237:LYS:O	2:B:241:ILE:HG23	2.16	0.45
2:E:208:LYS:HB3	2:E:208:LYS:NZ	2.32	0.45
2:B:87:LYS:HA	2:B:87:LYS:CE	2.47	0.45
2:B:217:LYS:O	2:B:218:GLU:HB2	2.16	0.45
3:C:131:ASP:O	3:C:135:LEU:HG	2.17	0.45
2:B:275:THR:HG23	2:B:280:MSE:HG3	1.99	0.45
2:B:247:ARG:HH11	2:B:247:ARG:HG3	1.82	0.44
2:B:175:ARG:HA	2:B:197:VAL:HG13	1.99	0.44
1:A:12:U:O2	1:A:14:U:H2'	2.17	0.44
2:E:229:THR:CG2	2:E:235:MSE:HE3	2.47	0.44
2:B:203:PHE:HB3	2:B:204:PRO:HD3	1.99	0.44
2:E:153:GLU:HG3	2:E:173:TYR:CE1	2.53	0.44
2:E:276:LYS:NZ	2:E:278:THR:CG2	2.80	0.44
2:E:268:TYR:C	2:E:269:LYS:HG2	2.38	0.44
2:B:224:LYS:HD2	4:B:436:HOH:O	2.17	0.44
2:E:88:LEU:CD1	2:E:106:LEU:HD13	2.48	0.44
3:C:169:PRO:HG3	3:C:193:ALA:HB1	2.00	0.44
2:B:322:MSE:HE2	2:B:322:MSE:HB2	1.90	0.44
2:E:108:ASN:O	2:E:112:LYS:HG3	2.18	0.44
2:E:88:LEU:HA	2:E:88:LEU:HD12	1.84	0.44
2:B:228:LEU:C	2:B:228:LEU:HD23	2.39	0.44
1:A:1:C:H2'	1:A:2:C:C5'	2.48	0.43
2:B:179:ASN:HB3	4:B:420:HOH:O	2.17	0.43
2:E:131:CYS:HB2	2:E:227:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:THR:HG22	3:C:149:ILE:N	2.33	0.43
2:B:308:ARG:C	2:B:308:ARG:HD3	2.34	0.43
2:B:286:MSE:CE	2:B:304:ARG:HB3	2.46	0.43
2:B:202:THR:OG1	2:B:205:GLN:HG3	2.19	0.43
3:C:146:LYS:HE2	3:C:151:TYR:OH	2.18	0.43
2:B:214:MSE:HB2	2:B:342:PRO:HG3	2.01	0.43
2:E:105:ARG:HH21	2:E:308:ARG:HD2	1.84	0.42
2:E:129:TYR:CD2	2:E:158:LEU:HD22	2.53	0.42
2:B:63:ASP:OD2	2:B:63:ASP:C	2.58	0.42
2:B:261:ARG:HG2	2:B:275:THR:CG2	2.49	0.42
2:B:79:MSE:HE1	2:B:87:LYS:CG	2.48	0.42
2:B:210:VAL:O	2:B:214:MSE:HG3	2.20	0.42
1:D:18:A:C2	1:D:19:G:C4	3.07	0.42
2:B:336:ILE:HD13	2:B:336:ILE:HA	1.85	0.42
3:C:176:LYS:HB3	3:C:178:TYR:CD2	2.55	0.42
2:E:171:GLN:O	2:E:172:GLN:HG2	2.20	0.42
3:C:138:ARG:HG2	3:C:183:TRP:CE2	2.55	0.41
2:B:259:ASN:HB2	2:B:320:GLU:OE1	2.20	0.41
2:B:308:ARG:NH1	2:B:312:ASP:OD1	2.52	0.41
2:B:247:ARG:HG3	2:B:247:ARG:NH1	2.35	0.41
2:E:132:ILE:CD1	2:E:303:ALA:HB2	2.49	0.41
3:C:195:HIS:O	3:C:198:ASP:N	2.48	0.41
1:D:10:C:P	4:D:106:HOH:O	2.78	0.41
1:D:16:A:H4'	2:E:73:ASN:HB2	2.01	0.41
2:E:193:THR:HG22	2:E:195:ASP:H	1.85	0.41
2:E:144:PRO:HA	2:E:145:PRO:HD3	1.78	0.41
2:E:275:THR:HG22	2:E:276:LYS:N	2.35	0.41
2:B:170:PHE:CD1	2:B:170:PHE:C	2.94	0.41
2:E:237:LYS:HB2	2:E:237:LYS:NZ	2.36	0.41
2:B:250:TYR:HA	2:B:251:PRO:HD3	1.87	0.41
2:E:305:ILE:HG22	2:E:309:MSE:HE2	2.03	0.41
2:B:221:THR:OG1	2:B:222:LYS:N	2.53	0.40
2:E:163:THR:OG1	2:E:165:GLU:HB2	2.21	0.40
2:B:131:CYS:SG	2:B:214:MSE:HE3	2.61	0.40
2:E:115:LEU:HD12	2:E:115:LEU:O	2.21	0.40
2:E:268:TYR:O	2:E:269:LYS:CB	2.69	0.40
3:C:170:LYS:HB3	3:C:170:LYS:HE2	1.95	0.40
4:A:108:HOH:O	3:C:191:LYS:HD3	2.21	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	B	270/303 (89%)	257 (95%)	13 (5%)	0	100	100
2	E	268/303 (88%)	261 (97%)	6 (2%)	1 (0%)	39	65
3	C	63/120 (52%)	57 (90%)	5 (8%)	1 (2%)	12	24
All	All	601/726 (83%)	575 (96%)	24 (4%)	2 (0%)	46	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	166	GLY
2	E	292	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	255/270 (94%)	243 (95%)	12 (5%)	32	59
2	E	253/270 (94%)	239 (94%)	14 (6%)	27	51
3	C	63/109 (58%)	62 (98%)	1 (2%)	70	89
All	All	571/649 (88%)	544 (95%)	27 (5%)	32	59

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	141	GLU

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Mol	Chain	Res	Type
2	B	154	PHE
2	B	155	PRO
2	B	158	LEU
2	B	159	LEU
2	B	163	THR
2	B	180	THR
2	B	181	GLN
2	B	241	ILE
2	B	248	LEU
2	B	260	ILE
2	B	348	ARG
3	C	176	LYS
2	E	82	GLU
2	E	88	LEU
2	E	115	LEU
2	E	154	PHE
2	E	158	LEU
2	E	180	THR
2	E	207	LEU
2	E	208	LYS
2	E	216	LEU
2	E	239	LEU
2	E	249	LYS
2	E	291	ARG
2	E	292	PRO
2	E	349	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	274	GLN
3	C	168	HIS
3	C	185	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	25/26 (96%)	1 (4%)	0
1	D	17/26 (65%)	1 (5%)	0
All	All	42/52 (80%)	2 (4%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	12	U
1	D	12	U

There are no RNA pucker outliers to report.

## 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](#)

There are no ligands in this entry.

## 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<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	26/26 (100%)	-0.44	0 100 100	28, 36, 64, 70	0
1	D	19/26 (73%)	0.80	3 (15%) 3 1	44, 86, 119, 120	0
2	B	266/303 (87%)	-0.14	5 (1%) 70 64	17, 33, 52, 68	0
2	E	264/303 (87%)	-0.05	5 (1%) 70 64	20, 34, 59, 70	0
3	C	67/120 (55%)	0.57	7 (10%) 8 5	23, 41, 76, 101	0
All	All	642/778 (82%)	-0.01	20 (3%) 52 45	17, 35, 67, 120	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	199	PRO	11.9
3	C	198	ASP	10.0
1	D	22	A	3.2
2	E	292	PRO	3.1
3	C	196	PHE	3.1
2	E	67	LYS	3.0
3	C	158	VAL	2.9
1	D	23	C	2.9
2	E	66	TYR	2.8
1	D	8	C	2.7
3	C	127	ASP	2.7
2	B	337	GLU	2.7
2	E	317	ARG	2.4
2	B	92	LYS	2.4
2	B	270	VAL	2.3
2	B	110	TYR	2.3
2	E	293	HIS	2.3
2	B	274	GLN	2.2
3	C	130	THR	2.1
3	C	167	ILE	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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.