



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:48 AM GMT

PDB ID : 2RFK  
Title : Substrate RNA Positioning in the Archaeal H/ACA Ribonucleoprotein Complex  
Authors : Liang, B.; Xue, S.; Terns, R.M.; Terns, M.P.; Li, H.; Southeast Collaboratory for Structural Genomics (SECSG)  
Deposited on : 2007-09-30  
Resolution : 2.87 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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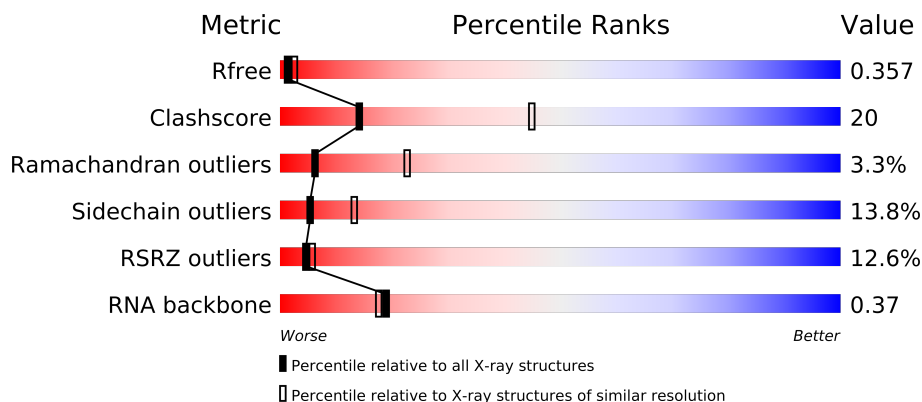
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.87 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))
$R_{free}$	66092	1360 (2.90-2.86)
Clashscore	79885	1696 (2.90-2.86)
Ramachandran outliers	78287	1647 (2.90-2.86)
Sidechain outliers	78261	1650 (2.90-2.86)
RSRZ outliers	66119	1362 (2.90-2.86)
RNA backbone	1838	1026 (3.36-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	D	21	
2	E	26	
3	F	14	
4	A	334	
5	B	53	
6	C	74	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5005 atoms, of which 0 are hydrogen and 0 are deuterium.

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 guide RNA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	21	Total	C	N	O	P	0	0	0
			450	201	86	143	20			

- Molecule 2 is a RNA chain called guide RNA 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	26	Total	C	N	O	P	0	0	0
			543	244	94	180	25			

- Molecule 3 is a RNA chain called target RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	14	Total	C	N	O	P	0	0	0
			300	134	54	99	13			

- Molecule 4 is a protein called Probable tRNA pseudouridine synthase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	334	Total	C	N	O	S	0	0	0
			2665	1716	466	473	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ALA	ASP	ENGINEERED	UNP Q7LWY0

- Molecule 5 is a protein called Ribosome biogenesis protein Nop10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	53	Total	C	N	O	S	0	0	0
			445	283	86	72	4			

- Molecule 6 is a protein called Small nucleolar rnp similar to gar1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	74	Total	C	N	O	S	0	0	0
			601	396	102	101	2			

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Zn	0	0
			1	1		

### 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.

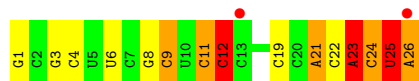
- Molecule 1: guide RNA 1

Chain D: 



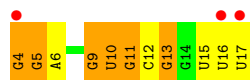
- Molecule 2: guide RNA 2

Chain E: 



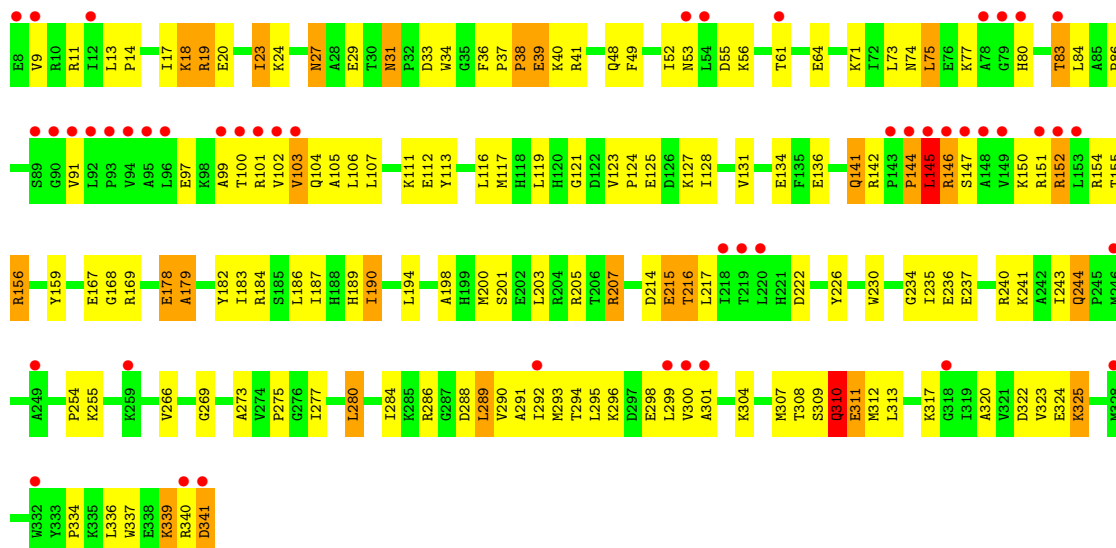
- Molecule 3: target RNA

Chain F: 



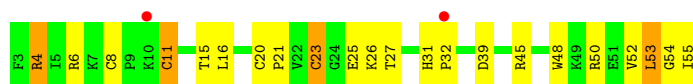
- Molecule 4: Probable tRNA pseudouridine synthase B

Chain A: 



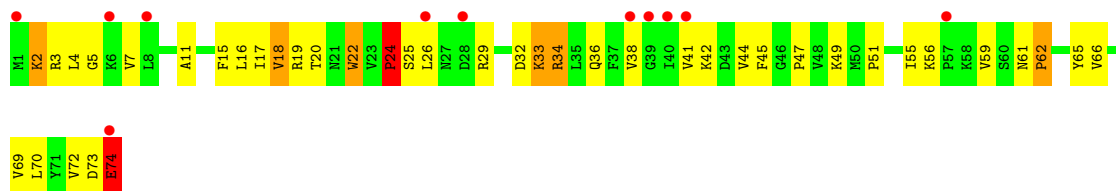
- Molecule 5: Ribosome biogenesis protein Nop10

Chain B: 



- Molecule 6: Small nucleolar rnp similar to gar1

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.56Å 96.56Å 240.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.52 – 2.87 38.04 – 2.79	Depositor EDS
% Data completeness (in resolution range)	80.0 (42.52-2.87) 75.5 (38.04-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.248 , 0.300 0.317 , 0.357	Depositor DCC
$R_{free}$ test set	1042 reflections (4.73%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.0	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , -1.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 24442 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5005	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: ZN

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	D	0.72	0/503	1.39	5/784 (0.6%)
2	E	0.80	0/604	1.51	7/938 (0.7%)
3	F	0.90	0/335	1.51	5/522 (1.0%)
4	A	0.55	1/2725 (0.0%)	0.67	0/3684
5	B	0.53	0/458	0.77	1/613 (0.2%)
6	C	1.33	3/615 (0.5%)	0.71	1/831 (0.1%)
All	All	0.75	4/5240 (0.1%)	0.99	19/7372 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	74	GLU	CD-OE1	21.63	1.49	1.25
6	C	74	GLU	CD-OE2	20.98	1.48	1.25
6	C	36	GLN	CD-OE1	5.33	1.35	1.24
4	A	145	LEU	C-N	5.17	1.46	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	74	GLU	OE1-CD-OE2	8.35	133.32	123.30
1	D	5	U	C3'-C2'-C1'	-7.72	95.32	101.50
3	F	4	G	P-O3'-C3'	6.72	127.76	119.70
5	B	23	CYS	CA-CB-SG	6.27	125.29	114.00
2	E	12	C	C3'-C2'-C1'	-6.09	96.63	101.50
1	D	5	U	P-O5'-C5'	-5.71	111.77	120.90
1	D	2	G	C6-C5-N7	-5.53	127.08	130.40
3	F	4	G	C3'-C2'-C1'	5.45	105.86	101.50
2	E	11	C	C4'-C3'-C2'	-5.45	97.15	102.60
2	E	9	C	C6-N1-C2	5.30	122.42	120.30
2	E	1	G	C3'-C2'-C1'	-5.15	97.38	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	G	C4'-C3'-C2'	-5.14	97.46	102.60
2	E	23	A	C1'-O4'-C4'	-5.14	105.79	109.90
3	F	6	A	O4'-C1'-N9	5.11	112.29	108.20
1	D	9	G	C1'-O4'-C4'	-5.09	105.83	109.90
2	E	25	U	C4'-C3'-C2'	-5.08	97.52	102.60
3	F	9	G	O4'-C1'-N9	-5.05	104.16	108.20
1	D	2	G	N1-C6-O6	5.05	122.93	119.90
3	F	5	G	C3'-C2'-C1'	-5.01	97.49	101.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	450	0	232	8	0
2	E	543	0	284	14	0
3	F	300	0	152	9	0
4	A	2665	0	2750	116	0
5	B	445	0	451	19	0
6	C	601	0	637	34	0
7	B	1	0	0	0	0
All	All	5005	0	4506	186	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (186) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:20:CYS:HB3	5:B:23:CYS:HB3	1.32	1.08
4:A:284:ILE:HB	4:A:309:SER:HB3	1.46	0.95
3:F:10:U:H4'	3:F:11:G:O5'	1.66	0.92
4:A:19:ARG:HH12	4:A:254:PRO:HB3	1.36	0.88
4:A:41:ARG:O	4:A:240:ARG:NH2	2.09	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:99:ALA:O	4:A:102:VAL:HG22	1.77	0.85
4:A:146:ARG:HH11	4:A:146:ARG:HA	1.40	0.84
6:C:20:THR:HG23	6:C:51:PRO:HD2	1.62	0.82
4:A:103:VAL:HA	4:A:106:LEU:HD12	1.64	0.80
4:A:80:HIS:HE1	4:A:83:THR:HB	1.50	0.76
4:A:142:ARG:CZ	4:A:154:ARG:HD2	2.14	0.76
4:A:117:MET:HG3	4:A:187:ILE:HG23	1.67	0.75
4:A:292:ILE:O	4:A:300:VAL:HG23	1.88	0.74
5:B:20:CYS:CB	5:B:23:CYS:HB3	2.13	0.73
4:A:141:GLN:HG2	4:A:156:ARG:HB2	1.72	0.72
4:A:144:PRO:HD2	6:C:25:SER:HA	1.72	0.72
4:A:307:MET:HE3	4:A:312:MET:HA	1.71	0.71
4:A:13:LEU:HB3	4:A:14:PRO:HD2	1.74	0.70
4:A:294:THR:OG1	4:A:298:GLU:HG2	1.93	0.69
4:A:307:MET:HE3	4:A:312:MET:HG2	1.75	0.69
4:A:73:LEU:HB3	4:A:75:LEU:HD13	1.74	0.69
6:C:22:TRP:CH2	6:C:72:VAL:HG11	2.29	0.68
2:E:23:A:N3	2:E:23:A:H2'	2.09	0.67
4:A:142:ARG:NH2	4:A:150:LYS:HE3	2.10	0.66
4:A:23:ILE:HD13	4:A:23:ILE:H	1.62	0.64
2:E:4:C:H4'	4:A:64:GLU:OE2	1.97	0.64
4:A:80:HIS:CE1	4:A:83:THR:HB	2.31	0.64
4:A:141:GLN:OE1	4:A:154:ARG:HB3	1.97	0.63
6:C:4:LEU:HD13	6:C:72:VAL:HB	1.80	0.63
6:C:4:LEU:HD12	6:C:22:TRP:CH2	2.34	0.63
5:B:39:ASP:OD1	5:B:45:ARG:NH2	2.32	0.62
6:C:11:ALA:HB2	6:C:17:ILE:HD11	1.80	0.62
4:A:286:ARG:NH1	4:A:307:MET:HA	2.15	0.62
6:C:22:TRP:CZ2	6:C:72:VAL:HG11	2.34	0.62
4:A:151:ARG:O	4:A:152:ARG:O	2.19	0.61
4:A:112:GLU:HB3	4:A:207:ARG:HB3	1.81	0.61
4:A:101:ARG:O	4:A:104:GLN:HG3	2.01	0.61
5:B:4:ARG:NH1	5:B:4:ARG:HB3	2.16	0.60
5:B:4:ARG:HB3	5:B:4:ARG:HH11	1.65	0.60
4:A:34:TRP:O	4:A:296:LYS:NZ	2.31	0.60
4:A:19:ARG:NH1	4:A:254:PRO:HB3	2.14	0.60
4:A:18:LYS:HE3	4:A:18:LYS:HA	1.82	0.59
4:A:80:HIS:HE1	4:A:83:THR:CB	2.15	0.59
6:C:7:VAL:CG2	6:C:70:LEU:HD23	2.32	0.59
4:A:84:LEU:HD11	4:A:205:ARG:CZ	2.32	0.59
4:A:37:PRO:HG2	4:A:40:LYS:HB3	1.84	0.58
6:C:15:PHE:HE2	6:C:42:LYS:HB2	1.68	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:24:LYS:HD3	4:A:313:LEU:HA	1.84	0.58
4:A:119:LEU:HD23	4:A:198:ALA:HB2	1.85	0.58
6:C:7:VAL:HG12	6:C:66:VAL:HA	1.86	0.58
2:E:25:U:H6	2:E:26:A:H4'	1.68	0.57
4:A:97:GLU:O	4:A:100:THR:HG23	2.04	0.57
6:C:2:LYS:HE3	6:C:2:LYS:H	1.69	0.57
4:A:186:LEU:O	4:A:190:ILE:HG22	2.04	0.57
1:D:1:G:HO5'	1:D:1:G:H8	1.53	0.57
5:B:50:ARG:HG2	5:B:55:ILE:HB	1.86	0.57
4:A:307:MET:HE2	4:A:320:ALA:HB2	1.87	0.57
4:A:73:LEU:HB3	4:A:75:LEU:CD1	2.35	0.56
4:A:308:THR:HB	4:A:311:GLU:HG3	1.87	0.56
1:D:15:G:H1	3:F:12:C:H42	1.52	0.56
1:D:14:C:H42	3:F:13:G:H1	1.52	0.56
4:A:334:PRO:O	4:A:336:LEU:HD12	2.05	0.56
2:E:21:A:H2'	2:E:21:A:N3	2.21	0.56
4:A:131:VAL:HG11	4:A:194:LEU:HD21	1.86	0.55
4:A:277:ILE:HG21	4:A:280:LEU:HD23	1.89	0.55
5:B:8:CYS:HB3	5:B:11:CYS:H	1.71	0.55
6:C:24:PRO:HD2	6:C:44:VAL:HG21	1.89	0.55
4:A:337:TRP:O	4:A:339:LYS:HG3	2.07	0.54
4:A:141:GLN:HG3	4:A:154:ARG:O	2.07	0.54
1:D:18:G:N2	2:E:4:C:O2	2.39	0.54
2:E:25:U:C6	2:E:26:A:H4'	2.42	0.54
4:A:117:MET:HG3	4:A:187:ILE:CG2	2.36	0.54
6:C:15:PHE:HA	6:C:55:ILE:O	2.08	0.54
4:A:38:PRO:O	4:A:40:LYS:N	2.38	0.53
6:C:4:LEU:HA	6:C:22:TRP:HZ3	1.73	0.53
4:A:291:ALA:HB1	4:A:293:MET:HE3	1.91	0.53
6:C:7:VAL:HG23	6:C:70:LEU:HD23	1.90	0.52
4:A:230:TRP:HA	4:A:235:ILE:H	1.73	0.52
6:C:73:ASP:OD2	6:C:74:GLU:N	2.42	0.52
6:C:15:PHE:CZ	6:C:56:LYS:HB2	2.44	0.52
6:C:22:TRP:HH2	6:C:72:VAL:HG11	1.75	0.52
4:A:289:LEU:HD12	4:A:304:LYS:NZ	2.25	0.52
4:A:38:PRO:O	4:A:41:ARG:HG2	2.10	0.52
6:C:4:LEU:HB3	6:C:70:LEU:O	2.10	0.52
4:A:141:GLN:CD	4:A:154:ARG:HB3	2.31	0.51
6:C:72:VAL:O	6:C:72:VAL:HG13	2.11	0.50
4:A:38:PRO:C	4:A:40:LYS:H	2.15	0.50
6:C:33:LYS:HE3	6:C:69:VAL:HB	1.92	0.50
4:A:77:LYS:HG2	4:A:100:THR:HG21	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:116:LEU:HD13	5:B:16:LEU:HD21	1.94	0.50
6:C:16:LEU:HD21	6:C:65:TYR:CD2	2.47	0.49
4:A:61:THR:HG22	4:A:86:PRO:HG3	1.94	0.49
4:A:124:PRO:HG2	4:A:127:LYS:HG3	1.92	0.49
6:C:65:TYR:HB3	6:C:70:LEU:HD21	1.95	0.49
2:E:25:U:H2'	2:E:26:A:C3'	2.43	0.49
4:A:48:GLN:HB3	4:A:49:PHE:CD2	2.48	0.49
4:A:183:ILE:HG21	4:A:203:LEU:HD22	1.94	0.48
5:B:45:ARG:O	5:B:48:TRP:HB3	2.13	0.48
4:A:214:ASP:C	4:A:216:THR:H	2.16	0.48
5:B:20:CYS:HB3	5:B:23:CYS:CB	2.23	0.48
6:C:4:LEU:HA	6:C:22:TRP:CZ3	2.49	0.48
4:A:284:ILE:CB	4:A:309:SER:HB3	2.32	0.47
4:A:73:LEU:CB	4:A:75:LEU:HD13	2.41	0.47
4:A:266:VAL:HG11	4:A:292:ILE:HD11	1.97	0.47
4:A:322:ASP:O	4:A:324:GLU:HG3	2.15	0.47
2:E:25:U:H2'	2:E:26:A:H3'	1.96	0.47
4:A:121:GLY:HA2	4:A:169:ARG:HH21	1.80	0.47
4:A:31:ASN:HD21	4:A:33:ASP:HB2	1.80	0.47
4:A:36:PHE:HB3	4:A:41:ARG:HB3	1.97	0.46
4:A:308:THR:HG22	4:A:310:GLN:HB3	1.97	0.46
2:E:23:A:OP2	4:A:317:LYS:NZ	2.46	0.46
3:F:9:G:H8	3:F:9:G:OP1	1.97	0.46
4:A:288:ASP:OD1	4:A:288:ASP:N	2.49	0.46
5:B:53:LEU:O	5:B:55:ILE:HG13	2.15	0.46
4:A:289:LEU:HD12	4:A:304:LYS:HZ3	1.81	0.46
4:A:38:PRO:HD3	4:A:298:GLU:HB3	1.97	0.46
4:A:292:ILE:HG13	4:A:292:ILE:O	2.15	0.46
6:C:5:GLY:O	6:C:69:VAL:HA	2.16	0.46
4:A:14:PRO:HD3	4:A:159:TYR:CE2	2.51	0.46
6:C:38:VAL:HG21	6:C:70:LEU:HD12	1.98	0.46
1:D:3:G:O2'	4:A:269:GLY:O	2.34	0.45
4:A:13:LEU:HB3	4:A:14:PRO:CD	2.40	0.44
4:A:339:LYS:HD3	4:A:341:ASP:OXT	2.16	0.44
4:A:123:VAL:HG11	4:A:194:LEU:HD22	1.99	0.44
2:E:24:C:H2'	4:A:340:ARG:HH21	1.81	0.44
6:C:45:PHE:CD1	6:C:45:PHE:N	2.85	0.44
4:A:146:ARG:HB3	4:A:147:SER:H	1.56	0.44
4:A:134:GLU:HG2	6:C:47:PRO:HG3	2.00	0.44
4:A:37:PRO:O	4:A:38:PRO:C	2.55	0.44
4:A:125:GLU:HA	4:A:128:ILE:HD12	1.99	0.44
4:A:144:PRO:HB2	4:A:145:LEU:H	1.63	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:23:A:H4'	2:E:24:C:O5'	2.17	0.43
4:A:187:ILE:O	4:A:190:ILE:HG23	2.18	0.43
4:A:23:ILE:CD1	4:A:23:ILE:H	2.30	0.43
1:D:12:A:H61	3:F:15:U:H3	1.65	0.43
3:F:15:U:O5'	3:F:15:U:H6	2.02	0.43
4:A:266:VAL:HG13	4:A:323:VAL:HG21	2.00	0.43
6:C:15:PHE:CE2	6:C:42:LYS:HB2	2.53	0.43
4:A:178:GLU:HG2	4:A:179:ALA:H	1.84	0.43
4:A:295:LEU:H	4:A:295:LEU:HD22	1.82	0.43
4:A:222:ASP:HB3	4:A:226:TYR:CE2	2.54	0.43
4:A:286:ARG:HH12	4:A:307:MET:HA	1.82	0.43
6:C:18:VAL:HG23	6:C:55:ILE:HD13	2.00	0.43
1:D:15:G:H1	3:F:12:C:N4	2.16	0.43
4:A:144:PRO:O	4:A:146:ARG:HD2	2.19	0.42
5:B:48:TRP:C	5:B:48:TRP:CD1	2.93	0.42
4:A:103:VAL:O	4:A:104:GLN:C	2.58	0.42
4:A:91:VAL:HG22	4:A:217:LEU:HD13	2.01	0.42
4:A:273:ALA:C	4:A:275:PRO:HD2	2.39	0.42
5:B:25:GLU:HB3	5:B:26:LYS:H	1.70	0.42
4:A:236:GLU:O	4:A:237:GLU:C	2.58	0.42
5:B:31:HIS:HD2	5:B:32:PRO:O	2.02	0.42
4:A:284:ILE:HB	4:A:309:SER:CB	2.33	0.42
5:B:15:THR:HG21	5:B:27:THR:HG21	2.00	0.42
4:A:27:ASN:H	4:A:27:ASN:ND2	2.17	0.42
5:B:39:ASP:CG	5:B:45:ARG:HH22	2.23	0.42
4:A:56:LYS:NZ	4:A:86:PRO:O	2.52	0.42
4:A:17:ILE:HG13	4:A:17:ILE:O	2.19	0.42
4:A:53:ASN:HD22	4:A:216:THR:CG2	2.32	0.42
6:C:41:VAL:HG12	6:C:42:LYS:N	2.35	0.42
4:A:116:LEU:HB3	4:A:201:SER:HB2	2.02	0.42
6:C:32:ASP:O	6:C:34:ARG:N	2.53	0.42
4:A:307:MET:CE	4:A:312:MET:HG2	2.46	0.41
2:E:8:G:H2'	2:E:9:C:C6	2.55	0.41
4:A:293:MET:HE2	4:A:299:LEU:HA	2.03	0.41
4:A:183:ILE:HG21	4:A:203:LEU:CD2	2.50	0.41
2:E:23:A:N3	2:E:23:A:C2'	2.81	0.41
4:A:307:MET:CE	4:A:312:MET:HA	2.46	0.41
4:A:243:ILE:HG22	4:A:244:GLN:O	2.20	0.41
4:A:178:GLU:HG2	4:A:179:ALA:N	2.35	0.41
4:A:301:ALA:HA	4:A:325:LYS:O	2.20	0.41
4:A:184:ARG:HG2	4:A:200:MET:CE	2.51	0.41
3:F:12:C:H2'	3:F:13:G:H8	1.86	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:55:ASP:CG	5:B:32:PRO:HG3	2.41	0.41
5:B:6:ARG:HD3	5:B:27:THR:OG1	2.21	0.41
4:A:11:ARG:O	4:A:11:ARG:HG3	2.21	0.41
5:B:20:CYS:HA	5:B:21:PRO:HD2	1.83	0.41
4:A:111:LYS:HB3	4:A:113:TYR:CE1	2.56	0.41
4:A:230:TRP:O	4:A:234:GLY:HA2	2.21	0.41
6:C:61:ASN:HA	6:C:62:PRO:HD3	1.87	0.41
4:A:38:PRO:HA	4:A:41:ARG:CZ	2.51	0.41
6:C:16:LEU:HB2	6:C:55:ILE:HB	2.02	0.40
4:A:339:LYS:HB2	4:A:340:ARG:H	1.78	0.40
4:A:311:GLU:OE2	4:A:311:GLU:C	2.60	0.40
1:D:17:G:H1'	3:F:11:G:N2	2.36	0.40
2:E:11:C:H2'	2:E:12:C:H6	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	
4	A	332/334 (99%)	281 (85%)	40 (12%)	11 (3%)	6	23
5	B	51/53 (96%)	43 (84%)	7 (14%)	1 (2%)	11	39
6	C	72/74 (97%)	60 (83%)	9 (12%)	3 (4%)	4	15
All	All	455/461 (99%)	384 (84%)	56 (12%)	15 (3%)	6	23

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	38	PRO
4	A	103	VAL
4	A	152	ARG
4	A	179	ALA
4	A	39	GLU
4	A	144	PRO

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Mol	Chain	Res	Type
4	A	145	LEU
4	A	168	GLY
5	B	54	GLY
6	C	24	PRO
4	A	105	ALA
6	C	33	LYS
6	C	62	PRO
4	A	310	GLN
4	A	215	GLU

### 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	
4	A	283/283 (100%)	244 (86%)	39 (14%)	5	13
5	B	48/48 (100%)	44 (92%)	4 (8%)	16	42
6	C	67/67 (100%)	55 (82%)	12 (18%)	2	6
All	All	398/398 (100%)	343 (86%)	55 (14%)	5	13

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	9	VAL
4	A	18	LYS
4	A	19	ARG
4	A	20	GLU
4	A	23	ILE
4	A	27	ASN
4	A	29	GLU
4	A	31	ASN
4	A	39	GLU
4	A	52	ILE
4	A	71	LYS
4	A	74	ASN
4	A	75	LEU
4	A	83	THR

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Mol	Chain	Res	Type
4	A	107	LEU
4	A	136	GLU
4	A	141	GLN
4	A	146	ARG
4	A	155	THR
4	A	156	ARG
4	A	167	GLU
4	A	178	GLU
4	A	182	TYR
4	A	189	HIS
4	A	190	ILE
4	A	207	ARG
4	A	215	GLU
4	A	216	THR
4	A	241	LYS
4	A	244	GLN
4	A	255	LYS
4	A	280	LEU
4	A	289	LEU
4	A	290	VAL
4	A	310	GLN
4	A	311	GLU
4	A	325	LYS
4	A	339	LYS
4	A	341	ASP
5	B	4	ARG
5	B	11	CYS
5	B	52	VAL
5	B	53	LEU
6	C	2	LYS
6	C	3	ARG
6	C	18	VAL
6	C	19	ARG
6	C	22	TRP
6	C	24	PRO
6	C	26	LEU
6	C	29	ARG
6	C	34	ARG
6	C	49	LYS
6	C	59	VAL
6	C	74	GLU

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



sidechains are listed below:

Mol	Chain	Res	Type
4	A	27	ASN
4	A	31	ASN
4	A	63	HIS
4	A	80	HIS
4	A	268	HIS
6	C	27	ASN
6	C	36	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	20/21 (95%)	7 (35%)	0
2	E	25/26 (96%)	9 (36%)	1 (4%)
3	F	14/14 (100%)	5 (35%)	2 (14%)
All	All	59/61 (96%)	21 (35%)	3 (5%)

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	3	G
1	D	5	U
1	D	8	G
1	D	10	A
1	D	12	A
1	D	15	G
1	D	18	G
2	E	6	U
2	E	12	C
2	E	19	C
2	E	21	A
2	E	22	C
2	E	23	A
2	E	24	C
2	E	25	U
2	E	26	A
3	F	5	G
3	F	11	G
3	F	13	G
3	F	16	U
3	F	17	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	23	A
3	F	4	G
3	F	10	U

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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.

## 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	D	21/21 (100%)	0.63	0 100 100	32, 51, 84, 87	0
2	E	26/26 (100%)	0.64	2 (7%) 13 16	41, 49, 73, 74	0
3	F	14/14 (100%)	1.22	3 (21%) 1 2	52, 83, 106, 117	0
4	A	334/334 (100%)	0.86	48 (14%) 3 4	24, 43, 58, 90	0
5	B	53/53 (100%)	0.55	2 (3%) 38 46	32, 46, 53, 56	0
6	C	74/74 (100%)	1.02	11 (14%) 3 4	29, 35, 40, 41	0
All	All	522/522 (100%)	0.84	66 (12%) 4 6	24, 43, 73, 117	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	9	VAL	5.9
6	C	28	ASP	4.6
4	A	8	GLU	4.4
4	A	148	ALA	4.0
4	A	145	LEU	3.9
6	C	57	PRO	3.8
6	C	38	VAL	3.8
3	F	16	U	3.7
4	A	149	VAL	3.6
6	C	39	GLY	3.5
6	C	26	LEU	3.5
4	A	151	ARG	3.4
4	A	99	ALA	3.2
6	C	6	LYS	3.2
6	C	40	ILE	3.2
3	F	4	G	3.2
4	A	152	ARG	3.1
4	A	12	ILE	3.1
4	A	340	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
4	A	93	PRO	3.1
6	C	41	VAL	3.1
4	A	301	ALA	3.1
4	A	83	THR	2.9
4	A	318	GLY	2.9
4	A	100	THR	2.8
4	A	300	VAL	2.8
4	A	246	MET	2.7
4	A	146	ARG	2.7
4	A	143	PRO	2.6
5	B	10	LYS	2.5
4	A	147	SER	2.5
4	A	91	VAL	2.5
4	A	90	GLY	2.5
4	A	341	ASP	2.4
4	A	102	VAL	2.4
4	A	79	GLY	2.4
4	A	144	PRO	2.4
4	A	95	ALA	2.4
6	C	1	MET	2.3
2	E	26	A	2.3
4	A	80	HIS	2.3
4	A	92	LEU	2.3
4	A	153	LEU	2.3
4	A	53	ASN	2.3
4	A	249	ALA	2.3
4	A	54	LEU	2.2
4	A	220	LEU	2.2
4	A	332	TRP	2.2
4	A	61	THR	2.2
4	A	101	ARG	2.2
4	A	89	SER	2.2
4	A	78	ALA	2.2
4	A	328	MET	2.1
4	A	94	VAL	2.1
4	A	96	LEU	2.1
4	A	218	ILE	2.1
4	A	219	THR	2.1
4	A	259	LYS	2.1
5	B	32	PRO	2.1
3	F	17	U	2.1
4	A	292	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
6	C	8	LEU	2.1
6	C	74	GLU	2.1
2	E	13	C	2.0
4	A	299	LEU	2.0
4	A	103	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	ZN	B	1	1/1	0.13	-0.72	56,56,56,56	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.