



# Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:41 pm BST

PDB ID : 1UN6  
Title : THE CRYSTAL STRUCTURE OF A ZINC FINGER - RNA COMPLEX  
REVEALS TWO MODES OF MOLECULAR RECOGNITION  
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Deposited on : 2003-09-04  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

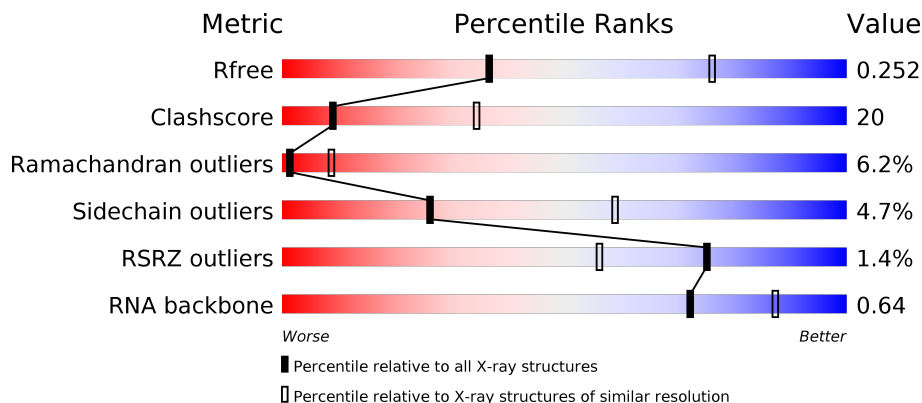
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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 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	B	87	 5% 36% 60%
1	C	87	 5% 43% 53%
1	D	87	 5% 8% 25% 33% 33%
2	E	61	 70% 26%

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Mol	Chain	Length	Quality of chain
2	F	61	 A horizontal bar chart representing the quality of chain. The bar is divided into two segments: a green segment on the left labeled '59%' and a yellow segment on the right labeled '38%'. The total length of the bar represents 100%.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	E	341	-	-	-	X
4	MG	F	304	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4554 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 TRANSCRIPTION FACTOR IIIA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	87	Total 713	C 451	N 133	O 121	S 8	0	0	1
1	C	87	Total 721	C 455	N 133	O 125	S 8	0	0	0
1	D	58	Total 475	C 299	N 86	O 85	S 5	0	0	0

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	61	Total 1304	C 582	N 240	O 422	P 60	0	0	0
2	F	61	Total 1304	C 582	N 240	O 422	P 60	0	0	0

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

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total 3	Mg 3	0	0
4	C	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	6	Total	Mg	0	0
			6	6		
4	E	2	Total	Mg	0	0
			2	2		

- Molecule 5 is water.

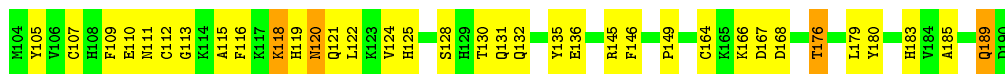
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			1	1		
5	C	1	Total	O	0	0
			1	1		
5	D	2	Total	O	0	0
			2	2		
5	E	3	Total	O	0	0
			3	3		
5	F	9	Total	O	0	0
			9	9		

### 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 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.

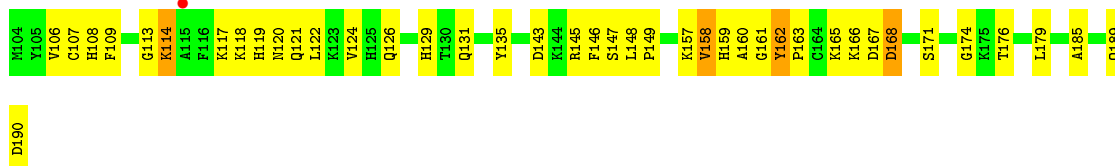
- Molecule 1: TRANSCRIPTION FACTOR IIIA

Chain B: 

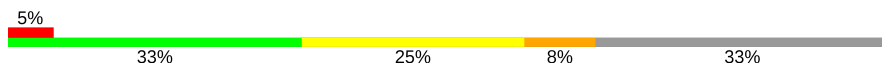


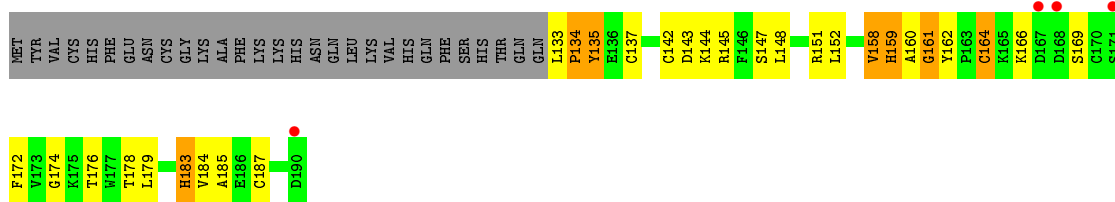
- Molecule 1: TRANSCRIPTION FACTOR IIIA

Chain C: 



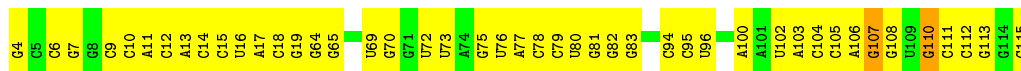
- Molecule 1: TRANSCRIPTION FACTOR IIIA

Chain D: 



- Molecule 2: 5S RIBOSOMAL RNA

Chain E: 



- Molecule 2: 5S RIBOSOMAL RNA

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.60Å 191.59Å 79.77Å 90.00° 101.51° 90.00°	Depositor
Resolution (Å)	35.19 – 3.10 35.19 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (35.19-3.10) 97.8 (35.19-3.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 3.12Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.216 , 0.259 0.213 , 0.252	Depositor DCC
$R_{free}$ test set	754 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.9	Xtrriage
Anisotropy	0.333	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 62.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4554	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	B	0.50	0/736	0.68	0/988
1	C	0.36	0/744	0.59	0/997
1	D	0.38	0/490	0.63	0/658
2	E	0.35	0/1458	0.67	0/2273
2	F	0.52	0/1458	0.67	0/2273
All	All	0.44	0/4886	0.66	0/7189

There are no bond length outliers.

There are no bond angle outliers.

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	B	713	0	679	40	0
1	C	721	0	683	35	0
1	D	475	0	452	31	0
2	E	1304	0	664	35	0
2	F	1304	0	664	22	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
4	F	6	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	F	9	0	0	0	0
All	All	4554	0	3142	155	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 20.

All (155) 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:B:176:THR:CG2	1:B:179:LEU:HD12	1.83	1.08
1:B:118:LYS:HB2	1:B:121:GLN:HE21	1.17	1.03
1:B:176:THR:HG23	1:B:179:LEU:HD12	1.03	1.00
1:D:158:VAL:HG12	1:D:159:HIS:H	1.27	0.98
1:C:118:LYS:H	1:C:121:GLN:HE21	1.09	0.93
2:E:112:C:H2'	2:E:113:G:H8	1.41	0.84
1:B:128:SER:HA	1:D:178:THR:HG23	1.62	0.80
1:B:118:LYS:H	1:B:121:GLN:NE2	1.81	0.79
1:C:107:CYS:HB3	1:C:122:LEU:HD11	1.63	0.78
1:D:158:VAL:O	1:D:160:ALA:N	2.18	0.77
1:B:118:LYS:HB3	1:B:120:ASN:ND2	2.00	0.77
2:E:112:C:H2'	2:E:113:G:C8	2.21	0.75
1:C:120:ASN:O	1:C:124:VAL:HG23	1.86	0.75
1:B:118:LYS:HB3	1:B:120:ASN:HD21	1.52	0.74
1:B:116:PHE:HZ	1:B:125:HIS:ND1	1.86	0.73
2:F:80:U:H2'	2:F:81:G:C8	2.24	0.73
2:E:76:U:H2'	2:E:77:A:H8	1.55	0.72
1:B:120:ASN:HD22	1:B:120:ASN:N	1.86	0.71
1:D:158:VAL:HG12	1:D:159:HIS:N	2.04	0.71
1:B:135:TYR:CZ	1:B:149:PRO:HG3	2.26	0.71
2:F:85:A:H2'	2:F:86:A:C8	2.27	0.70
1:D:161:GLY:HA3	1:D:174:GLY:O	1.93	0.69
1:D:176:THR:HG23	1:D:179:LEU:H	1.59	0.68
1:C:118:LYS:N	1:C:121:GLN:HE21	1.87	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:11:A:H4'	2:E:13:A:N7	2.10	0.65
2:E:6:C:H2'	2:E:7:G:C8	2.32	0.65
1:B:110:GLU:O	1:B:111:ASN:HB2	1.97	0.64
1:C:147:SER:HB2	1:C:148:LEU:HD12	1.79	0.64
2:E:72:U:O2'	2:E:73:U:H5'	1.98	0.64
1:D:142:CYS:SG	1:D:144:LYS:HG3	2.38	0.64
2:E:77:A:H2'	2:E:78:C:H5'	1.78	0.63
2:F:102:U:H2'	2:F:103:A:C8	2.33	0.63
1:B:136:GLU:HG2	1:B:145:ARG:NH1	2.16	0.61
1:B:120:ASN:HD22	1:B:120:ASN:H	1.48	0.61
1:B:118:LYS:HB2	1:B:121:GLN:NE2	2.02	0.60
1:C:148:LEU:HB3	1:C:149:PRO:HD2	1.82	0.60
1:C:118:LYS:H	1:C:121:GLN:NE2	1.92	0.60
1:D:164:CYS:SG	1:D:164:CYS:O	2.59	0.60
1:B:167:ASP:O	1:B:168:ASP:HB2	2.01	0.59
1:B:116:PHE:HZ	1:B:125:HIS:HD1	1.49	0.59
1:B:120:ASN:H	1:B:120:ASN:ND2	2.01	0.58
1:B:120:ASN:O	1:B:124:VAL:HG23	2.03	0.58
2:F:102:U:H2'	2:F:103:A:H8	1.67	0.58
2:E:110:G:H2'	2:E:111:C:H6	1.69	0.57
2:E:110:G:H2'	2:E:111:C:C6	2.39	0.57
1:B:120:ASN:N	1:B:120:ASN:ND2	2.52	0.57
1:D:159:HIS:O	1:D:160:ALA:HB3	2.04	0.57
1:D:134:PRO:HG2	1:D:135:TYR:H	1.70	0.56
1:C:119:HIS:CE1	2:E:75:G:C6	2.93	0.56
1:B:116:PHE:CZ	1:B:125:HIS:ND1	2.72	0.56
2:F:86:A:C5	2:F:94:C:H1'	2.41	0.56
1:D:158:VAL:C	1:D:160:ALA:H	2.07	0.56
2:E:77:A:C2'	2:E:78:C:H5'	2.35	0.56
2:E:80:U:H2'	2:E:81:G:O4'	2.06	0.56
1:D:134:PRO:HG2	1:D:135:TYR:CD2	2.42	0.55
1:C:148:LEU:N	1:C:148:LEU:HD12	2.21	0.55
2:E:15:C:O2'	2:E:16:U:H5'	2.07	0.55
2:E:103:A:H2'	2:E:104:C:C6	2.42	0.55
2:F:85:A:H2'	2:F:86:A:H8	1.72	0.54
2:E:104:C:H2'	2:E:105:C:C6	2.42	0.54
1:C:108:HIS:O	1:C:109:PHE:C	2.45	0.54
2:E:11:A:H4'	2:E:13:A:C5	2.43	0.53
1:C:189:GLN:O	1:C:190:ASP:HB2	2.09	0.53
2:E:95:C:O2'	2:E:96:U:H5'	2.08	0.53
1:B:135:TYR:O	1:B:145:ARG:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:VAL:HG13	1:C:113:GLY:O	2.10	0.52
1:B:115:ALA:C	1:B:116:PHE:CD2	2.83	0.52
1:C:167:ASP:OD1	1:C:168:ASP:N	2.43	0.52
1:B:164:CYS:SG	1:B:166:LYS:HB2	2.50	0.52
1:D:160:ALA:O	1:D:161:GLY:O	2.28	0.52
1:B:119:HIS:HE1	2:F:99:G:N7	2.08	0.52
1:C:161:GLY:O	1:C:162:TYR:HB2	2.10	0.51
2:E:107:G:O2'	2:E:108:G:H5'	2.09	0.51
2:E:81:G:N2	2:E:96:U:N3	2.58	0.51
1:D:148:LEU:HB2	1:D:151:ARG:HG3	1.93	0.50
2:E:4:G:H1	2:E:115:C:H42	1.59	0.50
2:E:78:C:H2'	2:E:79:C:C6	2.47	0.50
2:F:104:C:H2'	2:F:105:C:H6	1.76	0.50
1:C:117:LYS:HB3	1:C:121:GLN:HE22	1.77	0.50
1:C:120:ASN:ND2	2:E:75:G:O6	2.44	0.50
1:B:116:PHE:CD2	1:B:116:PHE:N	2.81	0.49
1:C:166:LYS:O	1:C:167:ASP:HB2	2.13	0.49
2:F:5:C:H42	2:F:114:G:H1	1.61	0.49
1:C:118:LYS:HA	2:E:75:G:N7	2.28	0.49
1:D:183:HIS:O	1:D:185:ALA:N	2.46	0.49
2:E:11:A:H4'	2:E:13:A:C8	2.48	0.49
1:D:133:LEU:CD2	1:D:147:SER:HB3	2.42	0.49
2:F:70:G:O2'	2:F:71:G:H5'	2.13	0.49
1:D:164:CYS:SG	1:D:166:LYS:HB2	2.53	0.48
1:D:164:CYS:C	1:D:166:LYS:H	2.17	0.48
1:B:176:THR:CG2	1:B:179:LEU:CD1	2.75	0.48
1:C:158:VAL:HG12	1:C:159:HIS:N	2.28	0.48
1:D:137:CYS:HA	1:D:152:LEU:HD11	1.95	0.48
2:F:100:A:H2'	2:F:101:A:O4'	2.14	0.48
1:B:118:LYS:HG3	2:F:75:G:C8	2.49	0.48
2:F:69:U:H2'	2:F:70:G:C8	2.49	0.47
1:C:161:GLY:O	1:C:174:GLY:O	2.33	0.47
1:C:113:GLY:O	1:C:114:LYS:C	2.53	0.47
1:C:158:VAL:C	1:C:160:ALA:H	2.17	0.47
1:B:145:ARG:C	1:B:146:PHE:CD1	2.89	0.46
2:F:70:G:H2'	2:F:71:G:H8	1.79	0.46
1:D:172:PHE:HD2	1:D:183:HIS:CE1	2.33	0.46
2:E:82:G:H2'	2:E:83:G:O4'	2.16	0.46
2:E:105:C:O2'	2:E:106:A:H5'	2.15	0.46
1:C:161:GLY:O	1:C:162:TYR:CB	2.63	0.46
1:B:118:LYS:N	1:B:121:GLN:NE2	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:70:G:H2'	2:F:71:G:C8	2.51	0.46
1:D:133:LEU:HD22	1:D:147:SER:HB3	1.97	0.45
1:C:158:VAL:C	1:C:160:ALA:N	2.70	0.45
2:E:82:G:H1	2:E:94:C:H42	1.63	0.45
2:E:69:U:H2'	2:E:70:G:C8	2.52	0.45
1:D:162:TYR:O	1:D:174:GLY:N	2.47	0.45
1:C:109:PHE:CZ	1:C:129:HIS:HB3	2.52	0.45
1:C:168:ASP:N	1:C:168:ASP:OD2	2.50	0.45
1:D:183:HIS:HD2	1:D:187:CYS:SG	2.40	0.45
1:D:147:SER:O	1:D:148:LEU:HD12	2.17	0.44
1:D:158:VAL:CG1	1:D:159:HIS:H	2.06	0.44
1:D:172:PHE:HD2	1:D:183:HIS:CG	2.36	0.44
1:B:107:CYS:HB2	1:B:122:LEU:CD1	2.47	0.44
1:C:163:PRO:HG2	1:C:165:LYS:HE3	1.99	0.44
2:E:64:G:O2'	2:E:65:G:H5'	2.16	0.44
2:E:9:C:H3'	2:E:10:C:C6	2.52	0.44
1:B:105:TYR:CE2	1:B:119:HIS:HB3	2.52	0.44
1:C:118:LYS:O	1:C:121:GLN:HG3	2.18	0.44
1:C:117:LYS:HB3	1:C:121:GLN:NE2	2.33	0.43
1:B:135:TYR:OH	1:B:149:PRO:HG3	2.18	0.43
2:F:80:U:H2'	2:F:81:G:H8	1.78	0.43
1:B:109:PHE:CD2	1:B:110:GLU:N	2.84	0.43
1:D:172:PHE:CD2	1:D:183:HIS:ND1	2.86	0.43
1:B:185:ALA:O	1:B:189:GLN:HG2	2.19	0.43
1:D:172:PHE:HD2	1:D:183:HIS:ND1	2.17	0.42
1:C:109:PHE:CE1	1:C:129:HIS:HB3	2.54	0.42
1:C:157:LYS:O	1:C:160:ALA:HB3	2.19	0.42
1:D:158:VAL:CG1	1:D:159:HIS:N	2.73	0.42
1:C:135:TYR:CE2	1:C:149:PRO:HD3	2.55	0.42
2:E:12:C:O2	2:E:12:C:C2'	2.68	0.42
2:F:68:C:H2'	2:F:69:U:C6	2.55	0.42
2:F:112:C:H2'	2:F:113:G:O4'	2.20	0.42
2:E:82:G:O2'	2:E:83:G:H5'	2.19	0.42
1:C:176:THR:OG1	1:C:179:LEU:HG	2.20	0.41
1:B:118:LYS:HG3	2:F:75:G:C5	2.55	0.41
1:B:118:LYS:CB	1:B:121:GLN:HE21	2.07	0.41
2:F:104:C:H2'	2:F:105:C:C6	2.56	0.41
2:F:16:U:H2'	2:F:18:C:C5	2.55	0.41
1:B:130:THR:O	1:B:131:GLN:CB	2.68	0.41
1:C:145:ARG:C	1:C:146:PHE:CD1	2.94	0.41
1:D:172:PHE:HE2	1:D:183:HIS:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:105:C:H2'	2:E:106:A:H8	1.86	0.41
1:B:118:LYS:HG3	2:F:75:G:N7	2.36	0.41
2:E:14:C:H6	2:E:14:C:O5'	2.04	0.41
2:E:102:U:H2'	2:E:103:A:O4'	2.21	0.41
1:B:180:TYR:O	1:B:183:HIS:HB3	2.22	0.40
1:C:185:ALA:O	1:C:189:GLN:NE2	2.55	0.40
1:D:159:HIS:O	1:D:160:ALA:CB	2.69	0.40
1:B:112:CYS:SG	1:B:113:GLY:N	2.94	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	B	85/87 (98%)	71 (84%)	14 (16%)	0	100	100
1	C	85/87 (98%)	70 (82%)	10 (12%)	5 (6%)	1	10
1	D	56/87 (64%)	40 (71%)	7 (12%)	9 (16%)	0	0
All	All	226/261 (87%)	181 (80%)	31 (14%)	14 (6%)	1	9

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	TYR
1	D	134	PRO
1	D	159	HIS
1	D	161	GLY
1	D	169	SER
1	C	131	GLN
1	C	143	ASP
1	D	135	TYR
1	D	158	VAL

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Mol	Chain	Res	Type
1	D	164	CYS
1	D	184	VAL
1	C	114	LYS
1	D	183	HIS
1	C	158	VAL

### 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	
1	B	79/80 (99%)	74 (94%)	5 (6%)	18	48
1	C	80/80 (100%)	77 (96%)	3 (4%)	33	66
1	D	53/80 (66%)	51 (96%)	2 (4%)	33	66
All	All	212/240 (88%)	202 (95%)	10 (5%)	26	59

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	118	LYS
1	B	120	ASN
1	B	132	GLN
1	B	176	THR
1	B	189	GLN
1	C	126	GLN
1	C	168	ASP
1	C	171	SER
1	D	143	ASP
1	D	145	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	108	HIS
1	B	119	HIS

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Mol	Chain	Res	Type
1	B	120	ASN
1	B	121	GLN
1	C	120	ASN
1	C	121	GLN
1	C	189	GLN
1	D	139	HIS
1	D	183	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	60/61 (98%)	6 (10%)	0
2	F	60/61 (98%)	4 (6%)	0
All	All	120/122 (98%)	10 (8%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	17	A
2	E	18	C
2	E	19	G
2	E	100	A
2	E	107	G
2	E	110	G
2	F	64	G
2	F	94	C
2	F	100	A
2	F	110	G

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](#)

Of 21 ligands modelled in this entry, 21 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 [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, 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	B	87/87 (100%)	-0.24	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	31, 53, 81, 88	0
1	C	87/87 (100%)	-0.04	1 (1%) <span style="border: 1px solid blue; padding: 2px;">80</span> <span style="border: 1px solid blue; padding: 2px;">64</span>	51, 94, 120, 126	0
1	D	58/87 (66%)	0.22	4 (6%) <span style="border: 1px solid red; padding: 2px;">16</span> <span style="border: 1px solid red; padding: 2px;">7</span>	62, 95, 136, 139	0
2	E	61/61 (100%)	0.07	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	66, 135, 159, 165	0
2	F	61/61 (100%)	-0.14	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	41, 63, 104, 123	0
All	All	354/383 (92%)	-0.04	5 (1%) <span style="border: 1px solid blue; padding: 2px;">75</span> <span style="border: 1px solid blue; padding: 2px;">56</span>	31, 82, 144, 165	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	171	SER	3.7
1	D	167	ASP	3.2
1	D	190	ASP	2.8
1	D	168	ASP	2.4
1	C	115	ALA	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	E	343	1/1	0.28	0.36	83,83,83,83	0
4	MG	C	344	1/1	0.58	0.24	69,69,69,69	0
4	MG	E	341	1/1	0.66	0.54	93,93,93,93	0
4	MG	B	308	1/1	0.72	0.11	62,62,62,62	0
4	MG	F	304	1/1	0.76	0.48	60,60,60,60	0
4	MG	B	306	1/1	0.83	0.12	83,83,83,83	0
4	MG	F	305	1/1	0.88	0.56	50,50,50,50	0
4	MG	C	342	1/1	0.92	0.62	53,53,53,53	0
4	MG	F	301	1/1	0.93	0.47	54,54,54,54	0
4	MG	F	303	1/1	0.93	0.28	61,61,61,61	0
4	MG	B	307	1/1	0.93	0.39	54,54,54,54	0
4	MG	F	302	1/1	0.93	0.75	59,59,59,59	0
4	MG	F	309	1/1	0.94	0.21	44,44,44,44	0
3	ZN	C	204	1/1	0.98	0.13	101,101,101,101	0
3	ZN	D	206	1/1	0.98	0.06	103,103,103,103	0
3	ZN	B	205	1/1	0.99	0.17	47,47,47,47	0
3	ZN	B	204	1/1	0.99	0.21	51,51,51,51	0
3	ZN	C	205	1/1	0.99	0.17	75,75,75,75	0
3	ZN	D	205	1/1	0.99	0.20	70,70,70,70	0
3	ZN	C	206	1/1	1.00	0.20	68,68,68,68	0
3	ZN	B	206	1/1	1.00	0.18	61,61,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.