



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:18 am GMT

PDB ID : 1UN6
Title : THE CRYSTAL STRUCTURE OF A ZINC FINGER - RNA COMPLEX
REVEALS TWO MODES OF MOLECULAR RECOGNITION
Authors : Lu, D.; Searles, M.A.; Klug, A.
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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

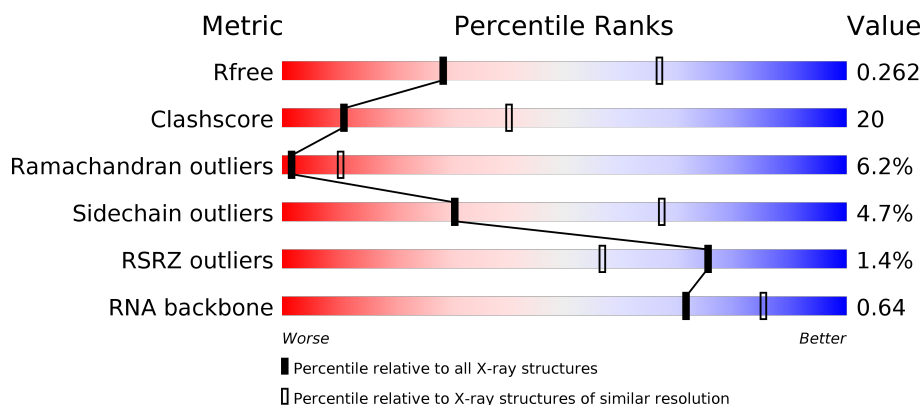
1 Overall quality at a glance

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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)
RNA backbone	2435	1112 (3.50-2.70)

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 $\leq 5\%$. 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	 60% 36% 5%
1	C	87	 53% 43% 5%
1	D	87	 5% 33% 25% 8% 33%
2	E	61	 26% 70% 5%

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Mol	Chain	Length	Quality of chain
2	F	61	 <div>59% 38%</div>

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	F	304	-	-	-	X

2 Entry composition

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
1	B	87	Total	C	N	O	S	0	0	1
			713	451	133	121	8			
1	C	87	Total	C	N	O	S	0	0	0
			721	455	133	125	8			
1	D	58	Total	C	N	O	S	0	0	0
			475	299	86	85	5			

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

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

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

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

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

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

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

- Molecule 5 is water.

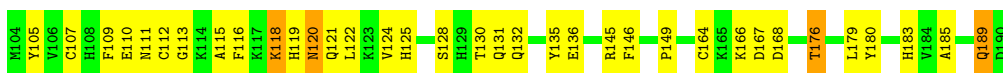
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	O 1	0	0
5	C	1	Total 1	O 1	0	0
5	D	2	Total 2	O 2	0	0
5	E	3	Total 3	O 3	0	0
5	F	9	Total 9	O 9	0	0

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 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.

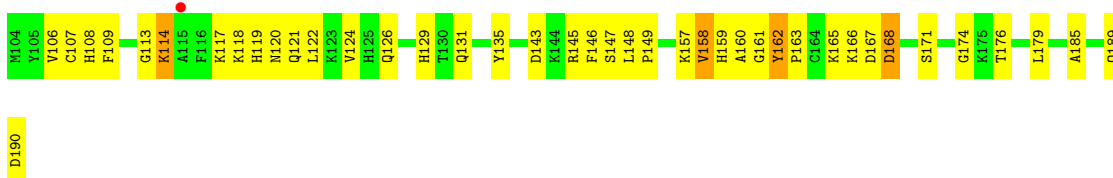
• Molecule 1: TRANSCRIPTION FACTOR IIIA

Chain B: 



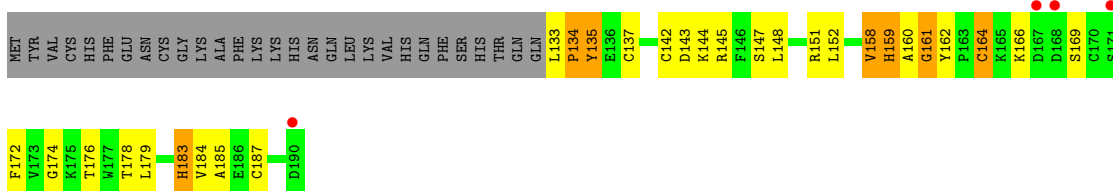
• Molecule 1: TRANSCRIPTION FACTOR IIIA

Chain C: 



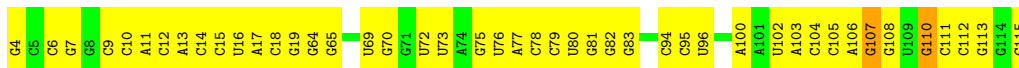
• Molecule 1: TRANSCRIPTION FACTOR IIIA

Chain D: 



• Molecule 2: 5S RIBOSOMAL RNA

Chain E: 



• Molecule 2: 5S RIBOSOMAL RNA

Chain F: 

G4	C5	U16	A17	C18	G19	G64	C68	U69	G70	G71	G75	U80	C81	A85	A86	C94	G99	A100	A101	U102	A103	C104	C105	G110	C111	C112	G113	G114	C115
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.259 0.213 , 0.262	Depositor DCC
R_{free} test set	754 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4554	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

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	
1	B	85/87 (98%)	71 (84%)	14 (16%)	0	100	100
1	C	85/87 (98%)	70 (82%)	10 (12%)	5 (6%)	2	12
1	D	56/87 (64%)	40 (71%)	7 (12%)	9 (16%)	0	0
All	All	226/261 (87%)	181 (80%)	31 (14%)	14 (6%)	2	10

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 ⓘ

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%)	21	56
1	C	80/80 (100%)	77 (96%)	3 (4%)	38	74
1	D	53/80 (66%)	51 (96%)	2 (4%)	38	74
All	All	212/240 (88%)	202 (95%)	10 (5%)	30	67

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 ⓘ

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 ⓘ

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 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	B	87/87 (100%)	-0.24	0	100	100	31, 53, 81, 88	0
1	C	87/87 (100%)	-0.03	1 (1%)	80	65	51, 94, 120, 126	0
1	D	58/87 (66%)	0.22	4 (6%)	18	7	62, 95, 136, 139	0
2	E	61/61 (100%)	0.07	0	100	100	66, 135, 159, 165	0
2	F	61/61 (100%)	-0.14	0	100	100	41, 63, 104, 123	0
All	All	354/383 (92%)	-0.04	5 (1%)	75	57	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. 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, 95th 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
4	MG	F	304	1/1	0.76	0.48	6.47	60,60,60,60	0
4	MG	C	344	1/1	0.58	0.24	1.13	69,69,69,69	0
3	ZN	B	204	1/1	0.99	0.21	0.80	51,51,51,51	0
3	ZN	C	206	1/1	1.00	0.20	0.53	68,68,68,68	0
3	ZN	D	205	1/1	0.99	0.20	-0.28	70,70,70,70	0
3	ZN	B	206	1/1	1.00	0.18	-0.28	61,61,61,61	0
3	ZN	C	205	1/1	0.99	0.17	-0.42	75,75,75,75	0
4	MG	B	308	1/1	0.72	0.11	-1.44	62,62,62,62	0
4	MG	B	306	1/1	0.83	0.12	-1.45	83,83,83,83	0
3	ZN	C	204	1/1	0.98	0.13	-1.98	101,101,101,101	0
4	MG	F	305	1/1	0.88	0.56	-	50,50,50,50	0
4	MG	F	301	1/1	0.93	0.47	-	54,54,54,54	0
4	MG	B	307	1/1	0.93	0.39	-	54,54,54,54	0
4	MG	C	342	1/1	0.92	0.62	-	53,53,53,53	0
4	MG	E	343	1/1	0.28	0.36	-	83,83,83,83	0
4	MG	F	303	1/1	0.93	0.27	-	61,61,61,61	0
3	ZN	D	206	1/1	0.98	0.06	-	103,103,103,103	0
4	MG	E	341	1/1	0.66	0.54	-	93,93,93,93	0
4	MG	F	309	1/1	0.94	0.21	-	44,44,44,44	0
3	ZN	B	205	1/1	0.99	0.17	-	47,47,47,47	0
4	MG	F	302	1/1	0.93	0.74	-	59,59,59,59	0

6.5 Other polymers

There are no such residues in this entry.