



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:25 am BST

PDB ID : 4P0Q  
Title : Crystal structure of Human Mus81-Eme1 in complex with 5'-flap DNA  
Authors : Gwon, G.H.; Baek, K.; Cho, Y.  
Deposited on : 2014-02-22  
Resolution : 2.85 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

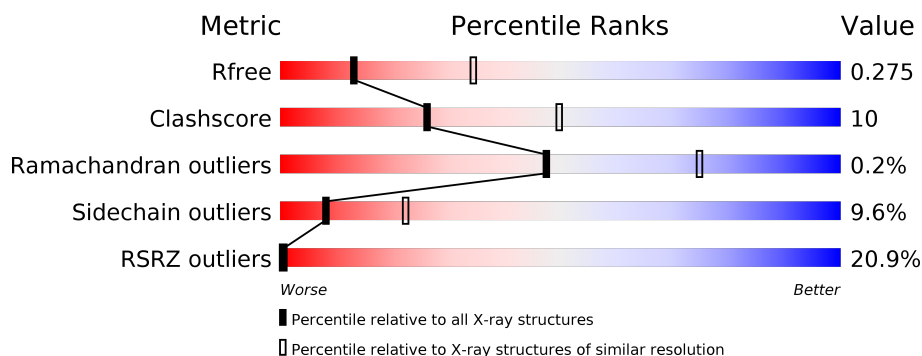
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	A	306	<div> <div>15%</div> <div>75%</div> <div>16%</div> <div>7%</div> </div>
2	B	393	<div> <div>15%</div> <div>48%</div> <div>21%</div> <div>28%</div> </div>
3	E	17	<div> <div>65%</div> <div>35%</div> <div>65%</div> </div>
4	F	6	<div> <div>83%</div> <div>33%</div> <div>67%</div> </div>
5	G	16	<div> <div>25%</div> <div>38%</div> <div>31%</div> <div>31%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5215 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 Crossover junction endonuclease MUS81.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2255	1414	422	411	8			

- Molecule 2 is a protein called Crossover junction endonuclease EME1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	284	Total	C	N	O	S	0	0	0
			2227	1401	397	415	14			

- Molecule 3 is a DNA chain called DNA GAATGTGTGTCTCAATC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	17	Total	C	N	O	P	0	0	0
			349	167	61	104	17			

- Molecule 4 is a DNA chain called DNA GGATTG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	6	Total	C	N	O	P	0	0	0
			127	60	24	37	6			

- Molecule 5 is a DNA chain called DNA TAACCAGACACACATT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	11	Total	C	N	O	P	0	0	0
			224	107	43	63	11			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		

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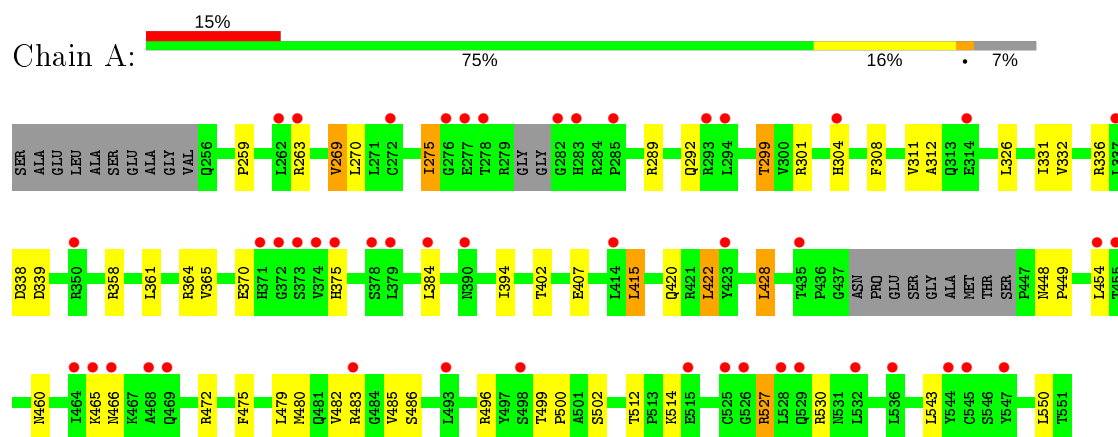
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	11	Total 11	O 11	0	0
6	E	1	Total 1	O 1	0	0
6	F	2	Total 2	O 2	0	0
6	G	1	Total 1	O 1	0	0

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

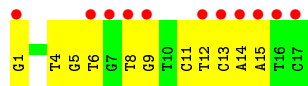
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Crossover junction endonuclease MUS81




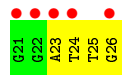
## ● Molecule 3: DNA GAATGTGTGTCTCAATC

Chain E: 



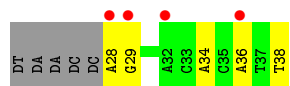
## ● Molecule 4: DNA GGATTG

Chain F: 



## ● Molecule 5: DNA TAACCAGACACACATT

Chain G: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.41Å 228.38Å 52.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.45 – 2.85 47.80 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.1 (42.45-2.85) 98.4 (47.80-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.243 , 0.276 0.247 , 0.275	Depositor DCC
$R_{free}$ test set	1269 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.6	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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](#)

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	0.23	0/2295	0.41	0/3103
2	B	0.23	0/2258	0.42	0/3054
3	E	0.49	0/390	0.93	1/600 (0.2%)
4	F	0.43	0/142	0.79	0/218
5	G	0.40	0/251	0.94	0/384
All	All	0.27	0/5336	0.53	1/7359 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	E	1	DG	C3'-C2'-C1'	-5.72	95.63	102.50

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	2255	0	2293	31	0
2	B	2227	0	2265	50	0
3	E	349	0	194	18	0
4	F	127	0	69	8	0
5	G	224	0	124	5	0
6	A	18	0	0	4	0
6	B	11	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1	0	0	2	0
6	F	2	0	0	0	0
6	G	1	0	0	0	0
All	All	5215	0	4945	105	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 10.

All (105) 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)
3:E:12:DT:H71	6:E:101:HOH:O	1.56	1.04
4:F:24:DT:H2''	4:F:25:DT:H5''	1.54	0.90
4:F:25:DT:H2''	4:F:26:DG:O5'	1.75	0.87
4:F:23:DA:H4'	4:F:24:DT:OP1	1.80	0.80
2:B:256:LEU:O	6:B:610:HOH:O	2.02	0.77
3:E:11:DC:C5	3:E:12:DT:H73	2.20	0.76
3:E:11:DC:C6	3:E:12:DT:H73	2.24	0.72
3:E:12:DT:C4	3:E:13:DC:C4	2.80	0.70
2:B:291:VAL:HG13	2:B:313:LEU:HB3	1.74	0.69
2:B:251:HIS:HB3	2:B:296:ARG:HG2	1.76	0.68
2:B:483:ARG:HA	2:B:501:VAL:HG21	1.76	0.66
1:A:289:ARG:NH2	1:A:292:GLN:OE1	2.29	0.66
3:E:6:DT:H3	5:G:34:DA:H61	1.45	0.65
2:B:524:GLN:HG3	2:B:551:ARG:HB2	1.79	0.65
4:F:25:DT:H4'	4:F:26:DG:OP1	1.97	0.64
1:A:486:SER:OG	5:G:34:DA:OP1	2.16	0.63
1:A:394:ILE:HD13	2:B:449:LYS:HD2	1.81	0.63
2:B:347:VAL:HG21	2:B:415:LEU:HD11	1.81	0.63
3:E:11:DC:C6	3:E:12:DT:C7	2.81	0.63
2:B:459:PHE:HA	2:B:462:GLU:HB2	1.82	0.62
4:F:23:DA:H2'	4:F:24:DT:H72	1.84	0.59
1:A:499:THR:HG21	2:B:560:LEU:HA	1.83	0.58
3:E:14:DA:H8	3:E:14:DA:H5''	1.69	0.58
3:E:12:DT:C7	6:E:101:HOH:O	2.29	0.57
2:B:241:LYS:HA	2:B:244:ARG:HD3	1.85	0.57
2:B:436:THR:N	6:B:609:HOH:O	2.27	0.57
1:A:308:PHE:HB2	1:A:332:VAL:HB	1.87	0.56
1:A:304:HIS:ND1	1:A:460:ASN:O	2.37	0.56
2:B:545:ILE:HG23	2:B:549:LEU:HD23	1.87	0.56
2:B:243:GLN:HB3	2:B:448:PHE:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:THR:HG21	1:A:301:ARG:HE	1.72	0.55
2:B:309:GLU:O	2:B:357:LYS:NZ	2.41	0.54
1:A:527:ARG:HD3	1:A:530:ARG:HB2	1.90	0.53
2:B:248:CYS:SG	6:B:608:HOH:O	2.59	0.52
2:B:404:SER:OG	2:B:407:ASP:OD2	2.28	0.52
1:A:336:ARG:NH2	1:A:370:GLU:OE2	2.41	0.52
2:B:283:GLU:N	6:B:610:HOH:O	2.43	0.51
3:E:12:DT:C5	3:E:13:DC:C4	2.99	0.51
2:B:483:ARG:NH1	2:B:487:GLN:OE1	2.44	0.51
3:E:8:DT:O4	3:E:9:DG:O6	2.30	0.50
2:B:238:THR:O	2:B:242:ALA:N	2.44	0.50
1:A:402:THR:HG23	1:A:407:GLU:HB2	1.94	0.50
2:B:344:GLN:O	2:B:348:THR:OG1	2.25	0.50
3:E:8:DT:C4	3:E:9:DG:C6	3.00	0.49
3:E:8:DT:O4	3:E:9:DG:C6	2.65	0.49
1:A:311:VAL:O	6:A:618:HOH:O	2.20	0.49
2:B:260:LEU:HB2	2:B:289:CYS:HA	1.94	0.49
1:A:499:THR:HG23	1:A:502:SER:H	1.77	0.49
2:B:253:ILE:HG22	2:B:279:ARG:HB2	1.94	0.49
1:A:472:ARG:HB2	2:B:562:PRO:HB2	1.95	0.49
2:B:347:VAL:O	2:B:351:THR:OG1	2.31	0.48
2:B:354:THR:HB	2:B:357:LYS:HD2	1.96	0.48
3:E:12:DT:C4	3:E:13:DC:N4	2.81	0.48
1:A:270:LEU:N	6:A:618:HOH:O	2.23	0.48
4:F:24:DT:H2''	4:F:25:DT:C5'	2.34	0.47
1:A:269:VAL:HG13	1:A:420:GLN:HG2	1.95	0.47
2:B:552:ARG:HD2	2:B:566:LEU:HB3	1.97	0.46
3:E:14:DA:H2'	3:E:15:DA:C8	2.49	0.46
2:B:529:ASP:OD1	2:B:544:ARG:NH2	2.47	0.46
1:A:480:MET:HG2	1:A:485:VAL:HG12	1.98	0.46
2:B:237:VAL:O	2:B:241:LYS:HG2	2.15	0.46
5:G:38:DT:H6	5:G:38:DT:H3'	1.81	0.45
3:E:8:DT:H5''	3:E:8:DT:H6	1.82	0.45
2:B:252:ILE:HD11	2:B:295:ARG:CZ	2.47	0.45
1:A:331:ILE:HB	1:A:361:LEU:HD23	1.99	0.45
2:B:362:VAL:HG11	2:B:432:LEU:HD23	1.98	0.45
4:F:24:DT:H2'	4:F:25:DT:H71	1.98	0.45
1:A:422:LEU:HD22	1:A:449:PRO:HB3	1.98	0.45
2:B:253:ILE:HG12	2:B:294:ARG:HB2	1.99	0.45
1:A:326:LEU:HD12	1:A:428:LEU:HB3	1.99	0.44
1:A:332:VAL:HG22	1:A:365:VAL:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:472:ASP:OD2	2:B:476:ARG:HB2	2.17	0.44
1:A:312:ALA:N	1:A:326:LEU:O	2.37	0.44
2:B:363:ILE:HB	2:B:425:ILE:HG12	2.00	0.43
2:B:446:ALA:O	2:B:450:LYS:HG2	2.19	0.43
3:E:8:DT:C4	3:E:9:DG:C5	3.06	0.43
2:B:354:THR:HB	2:B:357:LYS:HB2	1.99	0.43
1:A:543:LEU:HD23	2:B:478:LEU:HB3	2.01	0.43
1:A:448:ASN:HA	1:A:449:PRO:HA	1.79	0.42
1:A:496:ARG:O	1:A:496:ARG:NH2	2.52	0.42
2:B:258:PRO:HD3	6:B:610:HOH:O	2.18	0.42
1:A:415:LEU:HA	1:A:415:LEU:HD23	1.88	0.42
1:A:275:ILE:HG13	1:A:275:ILE:H	1.59	0.42
2:B:367:GLU:HG2	2:B:368:LYS:H	1.83	0.42
2:B:301:GLU:HG2	2:B:306:TRP:HZ2	1.84	0.42
5:G:28:DA:H2'	5:G:29:DG:O4'	2.20	0.42
1:A:270:LEU:O	6:A:618:HOH:O	2.22	0.42
1:A:338:ASP:OD2	1:A:339:ASP:N	2.53	0.42
3:E:4:DT:H3	5:G:36:DA:H61	1.68	0.42
1:A:512:THR:HG22	1:A:514:LYS:H	1.85	0.41
2:B:508:GLN:HA	2:B:511:VAL:HG12	2.02	0.41
2:B:422:GLN:HE21	2:B:422:GLN:HB2	1.52	0.41
2:B:473:LEU:HD12	2:B:473:LEU:H	1.85	0.41
1:A:475:PHE:CD1	1:A:500:PRO:HG3	2.55	0.41
2:B:321:PHE:HE1	2:B:343:LEU:HD11	1.86	0.41
2:B:490:ASN:O	2:B:552:ARG:NH2	2.53	0.41
1:A:311:VAL:N	6:A:618:HOH:O	2.47	0.41
2:B:519:SER:HB2	2:B:521:LYS:HD2	2.03	0.41
2:B:346:PHE:CZ	2:B:350:ILE:HD11	2.56	0.41
2:B:482:TRP:CE3	2:B:507:PRO:HG3	2.56	0.41
2:B:234:ALA:O	2:B:237:VAL:HG12	2.20	0.41
2:B:483:ARG:NH1	2:B:494:LEU:HD12	2.37	0.40
2:B:432:LEU:O	6:B:609:HOH:O	2.22	0.40
3:E:5:DG:H2''	3:E:6:DT:C6	2.55	0.40
4:F:25:DT:H6	4:F:25:DT:H5''	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	
1	A	279/306 (91%)	267 (96%)	11 (4%)	1 (0%)	34	62
2	B	276/393 (70%)	267 (97%)	9 (3%)	0	100	100
All	All	555/699 (79%)	534 (96%)	20 (4%)	1 (0%)	47	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/259 (95%)	227 (92%)	19 (8%)	13	32
2	B	242/334 (72%)	214 (88%)	28 (12%)	5	14
All	All	488/593 (82%)	441 (90%)	47 (10%)	8	22

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	ARG
1	A	269	VAL
1	A	275	ILE
1	A	299	THR
1	A	358	ARG

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Mol	Chain	Res	Type
1	A	364	ARG
1	A	375	HIS
1	A	384	LEU
1	A	415	LEU
1	A	422	LEU
1	A	428	LEU
1	A	454	LEU
1	A	465	LYS
1	A	466	ASN
1	A	479	LEU
1	A	482	VAL
1	A	483	ARG
1	A	527	ARG
1	A	550	LEU
2	B	238	THR
2	B	246	GLU
2	B	269	LEU
2	B	273	LEU
2	B	282	ILE
2	B	285	GLN
2	B	287	VAL
2	B	291	VAL
2	B	301	GLU
2	B	302	ASP
2	B	319	GLU
2	B	342	THR
2	B	344	GLN
2	B	351	THR
2	B	407	ASP
2	B	410	GLU
2	B	412	LEU
2	B	422	GLN
2	B	459	PHE
2	B	461	LEU
2	B	471	VAL
2	B	472	ASP
2	B	494	LEU
2	B	521	LYS
2	B	531	GLN
2	B	534	ARG
2	B	548	GLU
2	B	565	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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 ⓘ

There are no ligands in this entry.

## 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	A	285/306 (93%)	1.15	47 (16%) <b>1</b> <b>1</b>	31, 61, 114, 138	0
2	B	284/393 (72%)	1.28	59 (20%) <b>1</b> <b>0</b>	33, 65, 127, 148	0
3	E	17/17 (100%)	3.12	11 (64%) <b>0</b> <b>0</b>	64, 123, 170, 171	0
4	F	6/6 (100%)	4.01	5 (83%) <b>0</b> <b>0</b>	147, 156, 175, 177	0
5	G	11/16 (68%)	1.99	4 (36%) <b>0</b> <b>0</b>	109, 120, 144, 151	0
All	All	603/738 (81%)	1.31	126 (20%) <b>1</b> <b>0</b>	31, 64, 131, 177	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	542	SER	11.2
1	A	277	GLU	10.7
2	B	369	CYS	9.2
1	A	372	GLY	8.9
4	F	23	DA	8.2
2	B	234	ALA	8.1
2	B	541	THR	7.3
2	B	460	CYS	7.1
2	B	299	PRO	6.8
1	A	276	GLY	6.7
3	E	12	DT	6.6
3	E	7	DG	6.2
2	B	300	SER	6.0
1	A	532	LEU	6.0
2	B	298	GLY	5.9
2	B	243	GLN	5.8
2	B	306	TRP	5.7
1	A	526	GLY	5.6
1	A	466	ASN	5.6
3	E	17	DC	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	525	CYS	5.2
2	B	235	ALA	5.1
2	B	520	ASP	5.1
2	B	475	GLY	4.9
4	F	22	DG	4.9
2	B	461	LEU	4.7
1	A	285	PRO	4.6
2	B	516	GLN	4.6
1	A	435	THR	4.5
3	E	13	DC	4.3
1	A	374	VAL	4.3
3	E	15	DA	4.2
3	E	14	DA	4.1
2	B	297	ALA	4.1
1	A	378	SER	4.1
1	A	529	GLN	4.0
2	B	303	ARG	4.0
5	G	28	DA	4.0
4	F	26	DG	4.0
1	A	375	HIS	4.0
1	A	371	HIS	3.8
1	A	379	LEU	3.8
3	E	16	DT	3.8
2	B	465	TRP	3.8
1	A	544	TYR	3.7
3	E	1	DG	3.7
2	B	455	THR	3.6
2	B	245	PRO	3.6
2	B	526	LEU	3.6
3	E	8	DT	3.5
1	A	262	LEU	3.5
2	B	296	ARG	3.4
2	B	277	GLU	3.4
2	B	246	GLU	3.3
2	B	301	GLU	3.3
2	B	305	ASP	3.3
4	F	24	DT	3.2
2	B	294	ARG	3.2
1	A	465	LYS	3.2
2	B	494	LEU	3.2
1	A	278	THR	3.2
1	A	469	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	457	PHE	3.1
2	B	463	SER	3.1
2	B	458	SER	3.1
2	B	242	ALA	3.0
2	B	238	THR	3.0
2	B	329	LYS	3.0
1	A	515	GLU	3.0
1	A	528	LEU	2.9
2	B	240	MET	2.8
2	B	236	LEU	2.8
1	A	468	ALA	2.8
5	G	32	DA	2.8
2	B	448	PHE	2.8
1	A	454	LEU	2.8
2	B	489	LEU	2.7
1	A	283	HIS	2.7
3	E	9	DG	2.7
2	B	327	ASN	2.7
1	A	498	SER	2.7
1	A	373	SER	2.6
5	G	29	DG	2.6
1	A	350	ARG	2.5
2	B	554	TYR	2.5
1	A	483	ARG	2.5
2	B	530	ILE	2.5
1	A	536	LEU	2.5
3	E	6	DT	2.5
2	B	545	ILE	2.5
1	A	294	LEU	2.5
2	B	321	PHE	2.5
1	A	464	ILE	2.4
1	A	547	TYR	2.4
2	B	237	VAL	2.4
2	B	515	GLN	2.4
5	G	36	DA	2.4
2	B	527	LEU	2.4
1	A	423	TYR	2.3
1	A	293	ARG	2.3
2	B	368	LYS	2.3
1	A	455	THR	2.3
1	A	282	GLY	2.3
4	F	21	DG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	493	LEU	2.2
2	B	437	CYS	2.2
2	B	433	ALA	2.1
2	B	524	GLN	2.1
2	B	466	ALA	2.1
1	A	314	GLU	2.1
1	A	337	LEU	2.1
1	A	272	CYS	2.1
1	A	545	CYS	2.1
1	A	414	LEU	2.1
2	B	424	GLN	2.1
2	B	253	ILE	2.1
1	A	390	ASN	2.1
1	A	263	ARG	2.0
2	B	440	THR	2.0
1	A	304	HIS	2.0
2	B	425	ILE	2.0
1	A	384	LEU	2.0
2	B	370	PHE	2.0
2	B	459	PHE	2.0
2	B	438	ALA	2.0
2	B	415	LEU	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.