



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 12:16 AM EDT

PDB ID : 5WTI  
Title : Crystal structure of the CRISPR-associated protein in complex with crRNA and DNA  
Authors : Wu, D.; Guan, X.; Zhu, Y.; Huang, Z.  
Deposited on : 2016-12-13  
Resolution : 2.68 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.37.1
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)	:	2.37.1

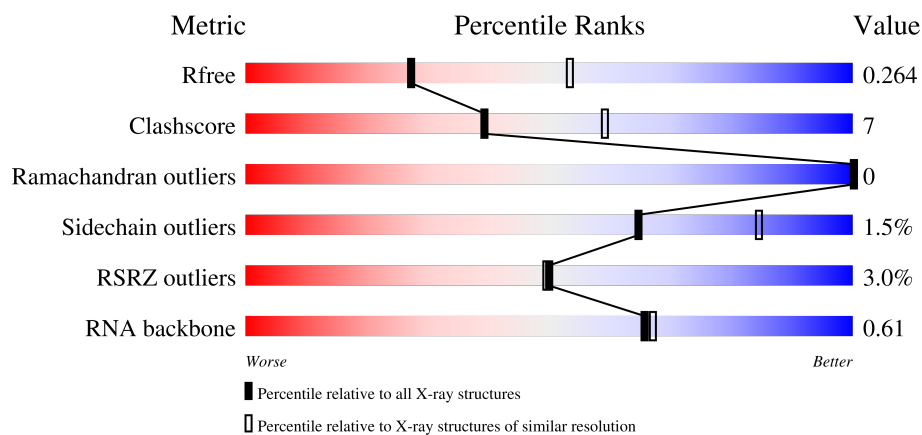
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)
RNA backbone	3102	1007 (2.98-2.38)

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 of 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	E	29	<div> <div>66%</div> <div>31%</div> <div>.</div> </div>
2	H	12	<div> <div>75%</div> <div>17%</div> <div>8%</div> </div>
3	Z	1108	<div> <div>3%</div> <div>71%</div> <div>17%</div> <div>11%</div> </div>
4	B	123	<div> <div>3%</div> <div>54%</div> <div>26%</div> <div>12%</div> <div>7%</div> </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
5	MG	B	202	-	-	-	X
5	MG	B	210	-	-	-	X
5	MG	B	211	-	-	-	X
5	MG	Z	1202	-	-	-	X
5	MG	Z	1205	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11276 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 DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	28	Total	C	N	O	P	0	0	0
			566	271	101	166	28			

- Molecule 2 is a DNA chain called DNA (5'-D(P\*GP\*TP\*GP\*TP\*GP\*GP\*AP\*TP\*TP\*CP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	11	Total	C	N	O	P	0	0	0
			227	108	39	69	11			

- Molecule 3 is a protein called CRISPR-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	982	Total	C	N	O	S	0	0	0
			7888	5044	1384	1440	20			

- Molecule 4 is a RNA chain called RNA (123-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	115	Total	C	N	O	P	0	0	0
			2462	1098	442	807	115			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	Z	5	Total	Mg	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	19	Total 19	Mg 19	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	10	Total 10	O 10	0	0
6	H	2	Total 2	O 2	0	0
6	Z	69	Total 69	O 69	0	0
6	B	26	Total 26	O 26	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

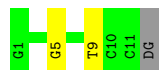
- Molecule 1: DNA (28-MER)

Chain E: 



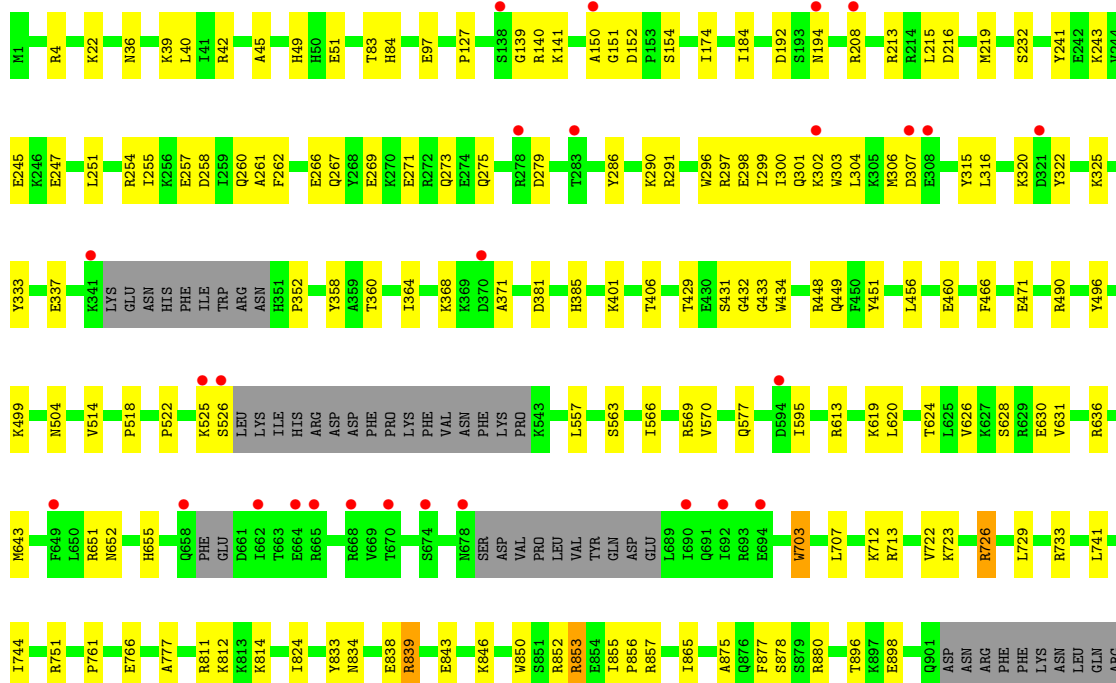
- Molecule 2: DNA (5'-D(P\*GP\*TP\*GP\*TP\*GP\*GP\*AP\*TP\*TP\*CP\*CP\*G)-3')

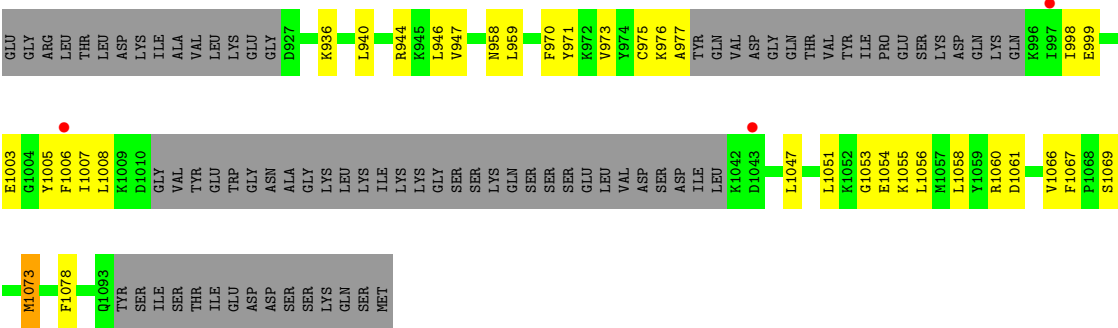
Chain H: 



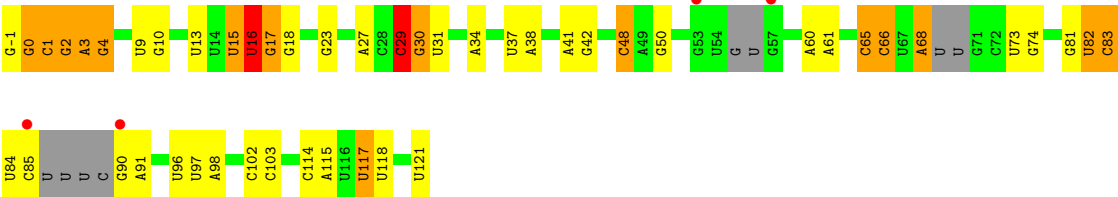
- Molecule 3: CRISPR-associated protein

Chain Z: 





● Molecule 4: RNA (123-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.06Å 138.74Å 95.61Å 90.00° 117.45° 90.00°	Depositor
Resolution (Å)	19.91 – 2.68 19.91 – 2.68	Depositor EDS
% Data completeness (in resolution range)	76.1 (19.91-2.68) 89.5 (19.91-2.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.67Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.217 , 0.264 0.216 , 0.264	Depositor DCC
$R_{free}$ test set	2000 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.1	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	11276	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: 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	E	0.59	0/633	0.92	0/972
2	H	0.61	0/253	1.02	0/389
3	Z	0.30	0/8058	0.47	1/10857 (0.0%)
4	B	0.28	0/2751	0.84	5/4281 (0.1%)
All	All	0.33	0/11695	0.63	6/16499 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	29	C	N3-C2-O2	-7.14	116.90	121.90
3	Z	194	ASN	C-N-CA	7.07	139.36	121.70
4	B	29	C	C2-N1-C1'	5.68	125.05	118.80
4	B	29	C	N1-C2-O2	5.57	122.24	118.90
4	B	16	U	N3-C2-O2	-5.32	118.47	122.20
4	B	16	U	C2-N1-C1'	5.14	123.86	117.70

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	E	566	0	316	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	227	0	126	2	0
3	Z	7888	0	7706	121	0
4	B	2462	0	1240	37	0
5	B	19	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
5	Z	5	0	0	0	0
6	B	26	0	0	1	0
6	E	10	0	0	0	0
6	H	2	0	0	0	0
6	Z	69	0	0	0	1
All	All	11276	0	9388	150	1

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 7.

All (150) 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:Z:651:ARG:NH1	4:B:117:U:OP1	2.10	0.84
4:B:-1:G:H1	4:B:29:C:H5	1.30	0.78
4:B:85:C:H5	4:B:90:G:H1	1.30	0.77
1:E:23:DT:H5''	3:Z:141:LYS:HG2	1.66	0.76
3:Z:254:ARG:CZ	3:Z:257:GLU:HG3	2.19	0.73
3:Z:216:ASP:HA	3:Z:219:MET:HE2	1.69	0.73
3:Z:557:LEU:HD13	3:Z:566:ILE:HD11	1.74	0.68
3:Z:940:LEU:HD12	3:Z:1066:VAL:HG12	1.75	0.68
3:Z:834:ASN:O	3:Z:839:ARG:NH1	2.27	0.68
2:H:5:DG:OP2	3:Z:401:LYS:NZ	2.26	0.68
3:Z:456:LEU:HD23	3:Z:466:PHE:HB3	1.79	0.64
3:Z:299:ILE:O	3:Z:302:LYS:HB2	1.98	0.64
4:B:0:G:H2'	4:B:1:C:O4'	1.97	0.64
3:Z:245:GLU:OE1	3:Z:368:LYS:NZ	2.28	0.62
3:Z:258:ASP:OD1	3:Z:260:GLN:HG2	2.00	0.62
3:Z:298:GLU:OE1	3:Z:322:TYR:OH	2.15	0.62
3:Z:431:SER:N	3:Z:432:GLY:HA2	2.16	0.61
3:Z:613:ARG:NH1	4:B:17:G:N7	2.49	0.61
3:Z:761:PRO:HB3	3:Z:766:GLU:HB3	1.82	0.60
3:Z:300:ILE:HG13	3:Z:304:LEU:HD12	1.83	0.60
4:B:73:U:H2'	4:B:74:G:C8	2.36	0.60
4:B:15:U:H4'	4:B:16:U:O5'	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:499:LYS:HB3	3:Z:504:ASN:HB3	1.84	0.59
4:B:73:U:H2'	4:B:74:G:H8	1.67	0.59
3:Z:275:GLN:NE2	3:Z:279:ASP:OD2	2.33	0.59
3:Z:152:ASP:OD1	3:Z:154:SER:OG	2.19	0.59
3:Z:976:LYS:HA	3:Z:1055:LYS:HD3	1.83	0.59
3:Z:269:GLU:O	3:Z:273:GLN:HG3	2.03	0.57
3:Z:518:PRO:HB3	3:Z:865:ILE:HA	1.87	0.57
3:Z:255:ILE:HD11	3:Z:358:TYR:HD1	1.70	0.57
3:Z:258:ASP:OD1	3:Z:261:ALA:N	2.18	0.57
3:Z:703:TRP:NE1	3:Z:707:LEU:HD11	2.20	0.56
1:E:7:DT:H2'	1:E:8:DG:C8	2.40	0.56
3:Z:875:ALA:HB2	3:Z:959:LEU:HD21	1.86	0.55
3:Z:570:VAL:HG22	3:Z:824:ILE:HB	1.88	0.55
3:Z:855:ILE:HB	3:Z:856:PRO:HD3	1.88	0.55
3:Z:577:GLN:N	3:Z:577:GLN:OE1	2.38	0.54
3:Z:51:GLU:OE1	3:Z:385:HIS:NE2	2.28	0.54
3:Z:1060:ARG:HH21	3:Z:1069:SER:HB3	1.72	0.54
1:E:14:DT:OP2	3:Z:857:ARG:NH2	2.41	0.54
3:Z:733:ARG:NH1	4:B:48:C:OP2	2.39	0.54
4:B:34:A:H62	4:B:73:U:H3	1.55	0.54
3:Z:49:HIS:NE2	3:Z:51:GLU:OE1	2.29	0.53
3:Z:36:ASN:HD22	3:Z:39:LYS:HE3	1.73	0.53
2:H:9:DT:O4'	3:Z:139:GLY:HA3	2.08	0.53
3:Z:406:THR:HG21	3:Z:460:GLU:HG3	1.90	0.52
3:Z:448:ARG:NH2	3:Z:471:GLU:OE1	2.34	0.52
3:Z:273:GLN:HG2	3:Z:286:TYR:HB3	1.92	0.52
3:Z:306:MET:O	3:Z:315:TYR:OH	2.18	0.52
3:Z:297:ARG:O	3:Z:301:GLN:NE2	2.41	0.50
3:Z:22:LYS:HE3	3:Z:434:TRP:CE2	2.47	0.50
3:Z:83:THR:HG22	3:Z:84:HIS:H	1.76	0.50
3:Z:970:PHE:CE2	3:Z:1006:PHE:HB2	2.47	0.50
3:Z:254:ARG:NH1	3:Z:257:GLU:HG3	2.26	0.50
3:Z:975:CYS:HB3	3:Z:998:ILE:HG22	1.93	0.49
3:Z:97:GLU:HG2	3:Z:174:ILE:HD11	1.94	0.49
3:Z:251:LEU:HD12	3:Z:364:ILE:HD12	1.93	0.49
3:Z:255:ILE:HD11	3:Z:358:TYR:CD1	2.47	0.49
3:Z:192:ASP:OD1	3:Z:213:ARG:NH2	2.36	0.48
3:Z:636:ARG:NH2	3:Z:729:LEU:O	2.38	0.48
4:B:9:U:H2'	4:B:10:G:C8	2.48	0.48
3:Z:852:ARG:HG2	3:Z:853:ARG:HG2	1.94	0.48
3:Z:150:ALA:N	3:Z:151:GLY:HA2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:296:TRP:CH2	3:Z:300:ILE:HD13	2.49	0.47
3:Z:1073:MET:HG3	3:Z:1078:PHE:HB2	1.96	0.47
4:B:82:U:H2'	4:B:83:C:C6	2.49	0.47
3:Z:241:TYR:CE1	3:Z:371:ALA:HB1	2.49	0.47
3:Z:290:LYS:HD3	3:Z:360:THR:HG22	1.96	0.47
3:Z:267:GLN:O	3:Z:271:GLU:HG3	2.14	0.47
3:Z:352:PRO:HB2	3:Z:1051:LEU:HD13	1.96	0.47
3:Z:843:GLU:HG3	3:Z:846:LYS:HE3	1.95	0.47
3:Z:4:ARG:O	3:Z:514:VAL:HG12	2.15	0.47
1:E:17:DC:OP1	3:Z:232:SER:OG	2.27	0.47
3:Z:297:ARG:HD3	3:Z:1047:LEU:CD1	2.45	0.47
3:Z:619:LYS:HD3	3:Z:624:THR:HG22	1.96	0.47
4:B:82:U:O2'	4:B:83:C:OP1	2.33	0.47
3:Z:563:SER:O	3:Z:569:ARG:NH2	2.48	0.47
3:Z:262:PHE:O	3:Z:266:GLU:HG3	2.15	0.46
3:Z:652:ASN:HA	3:Z:655:HIS:HB3	1.96	0.46
3:Z:316:LEU:HD21	3:Z:333:TYR:HE1	1.79	0.46
3:Z:878:SER:O	3:Z:958:ASN:ND2	2.40	0.46
3:Z:999:GLU:OE2	3:Z:1005:TYR:OH	2.25	0.46
4:B:82:U:H2'	4:B:83:C:H6	1.80	0.46
3:Z:643:MET:SD	3:Z:722:VAL:HG12	2.55	0.46
3:Z:303:TRP:O	3:Z:307:ASP:HB3	2.16	0.46
3:Z:522:PRO:O	3:Z:525:LYS:HD2	2.16	0.46
4:B:16:U:O2'	4:B:17:G:OP1	2.25	0.46
1:E:8:DG:H2'	1:E:9:DA:C8	2.52	0.45
3:Z:297:ARG:HD3	3:Z:1047:LEU:HD11	1.98	0.45
3:Z:846:LYS:O	3:Z:850:TRP:HB2	2.16	0.45
3:Z:42:ARG:NH2	3:Z:45:ALA:O	2.49	0.45
3:Z:628:SER:O	3:Z:631:VAL:HG22	2.16	0.45
3:Z:243:LYS:O	3:Z:247:GLU:HG3	2.16	0.45
3:Z:1054:GLU:O	3:Z:1055:LYS:HG2	2.17	0.45
4:B:65:C:HO2'	4:B:66:C:P	2.39	0.45
3:Z:877:PHE:HD1	3:Z:880:ARG:HG3	1.82	0.45
4:B:3:A:H2'	4:B:4:G:O4'	2.16	0.45
3:Z:215:LEU:O	3:Z:219:MET:HG3	2.17	0.44
3:Z:741:LEU:HD23	3:Z:744:ILE:HD12	1.99	0.44
3:Z:316:LEU:HD13	3:Z:337:GLU:HA	1.98	0.44
3:Z:944:ARG:HB3	3:Z:944:ARG:NH2	2.32	0.44
3:Z:620:LEU:O	4:B:3:A:H5''	2.17	0.44
3:Z:973:VAL:HG23	3:Z:1058:LEU:HB2	2.00	0.44
3:Z:1061:ASP:HB3	3:Z:1067:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:325:LYS:HE3	3:Z:325:LYS:HB3	1.82	0.44
3:Z:297:ARG:HG3	3:Z:301:GLN:NE2	2.32	0.44
3:Z:429:THR:OG1	3:Z:433:GLY:N	2.50	0.44
3:Z:971:TYR:HA	3:Z:1060:ARG:HG2	1.98	0.44
3:Z:36:ASN:O	3:Z:40:LEU:HG	2.19	0.43
3:Z:1007:ILE:HG13	3:Z:1008:LEU:HD22	1.98	0.43
1:E:21:DA:H1'	3:Z:140:ARG:HH11	1.84	0.43
3:Z:977:ALA:HA	3:Z:998:ILE:HA	2.00	0.43
4:B:-1:G:N1	4:B:29:C:H5	2.06	0.43
4:B:65:C:O2'	4:B:66:C:OP1	2.34	0.43
3:Z:940:LEU:HD23	3:Z:946:LEU:HA	2.01	0.43
3:Z:1053:GLY:HA2	3:Z:1056:LEU:CD2	2.49	0.43
4:B:50:G:O2'	6:B:301:HOH:O	2.21	0.43
3:Z:300:ILE:HG13	3:Z:304:LEU:CD1	2.49	0.43
3:Z:812:LYS:O	3:Z:814:LYS:HG3	2.19	0.43
4:B:9:U:H2'	4:B:10:G:H8	1.84	0.43
4:B:84:U:H3	4:B:91:A:H61	1.66	0.42
3:Z:208:ARG:H	3:Z:208:ARG:HG3	1.53	0.42
1:E:5:DA:H2'	1:E:6:DA:C8	2.54	0.42
3:Z:496:TYR:HB3	3:Z:499:LYS:HB2	2.02	0.42
3:Z:127:PRO:HB3	3:Z:184:ILE:HG22	2.01	0.42
3:Z:811:ARG:HA	4:B:27:A:H1'	2.02	0.42
3:Z:83:THR:HG22	3:Z:84:HIS:N	2.34	0.41
3:Z:947:VAL:HG23	4:B:13:U:H5'	2.02	0.41
3:Z:320:LYS:HZ2	4:B:121:U:HO3'	1.57	0.41
4:B:29:C:O2'	4:B:30:G:OP2	2.34	0.41
3:Z:626:VAL:O	3:Z:630:GLU:HG2	2.21	0.41
4:B:114:C:H2'	4:B:115:A:C8	2.56	0.41
3:Z:451:TYR:OH	4:B:96:U:OP1	2.30	0.41
3:Z:723:LYS:HD2	4:B:60:A:OP1	2.20	0.41
3:Z:291:ARG:HG2	3:Z:838:GLU:HA	2.03	0.41
4:B:2:G:H4'	4:B:3:A:OP1	2.21	0.41
3:Z:251:LEU:HD23	3:Z:251:LEU:HA	1.88	0.41
3:Z:449:GLN:HG3	4:B:102:C:C4	2.55	0.41
3:Z:726:ARG:NE	4:B:61:A:OP1	2.54	0.41
3:Z:1053:GLY:HA2	3:Z:1056:LEU:HD23	2.03	0.41
3:Z:944:ARG:HB3	3:Z:944:ARG:HH21	1.85	0.41
4:B:37:U:H5	4:B:68:A:N7	2.18	0.41
3:Z:525:LYS:O	3:Z:526:SER:HB2	2.20	0.41
3:Z:595:ILE:H	3:Z:595:ILE:HD12	1.86	0.41
4:B:34:A:C8	4:B:74:G:C2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:81:G:C6	4:B:82:U:C4	3.10	0.40
3:Z:300:ILE:HD12	3:Z:303:TRP:HB2	2.02	0.40
3:Z:751:ARG:NH1	3:Z:777:ALA:HB3	2.36	0.40
3:Z:896:THR:C	3:Z:898:GLU:H	2.25	0.40
4:B:16:U:H3'	4:B:16:U:O2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:1332:HOH:O	6:Z:1332:HOH:O[2_859]	2.19	0.01

## 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	
3	Z	966/1108 (87%)	931 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
3	Z	815/1005 (81%)	803 (98%)	12 (2%)	65	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Z	381	ASP
3	Z	490	ARG
3	Z	703	TRP
3	Z	712	LYS
3	Z	713	ARG
3	Z	726	ARG
3	Z	833	TYR
3	Z	839	ARG
3	Z	853	ARG
3	Z	936	LYS
3	Z	1003	GLU
3	Z	1073	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	Z	24	HIS
3	Z	36	ASN
3	Z	267	GLN
3	Z	273	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	B	111/123 (90%)	22 (19%)	10 (9%)

All (22) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	B	1	C
4	B	2	G
4	B	3	A
4	B	4	G
4	B	15	U
4	B	16	U
4	B	17	G
4	B	18	G
4	B	23	G
4	B	30	G

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Mol	Chain	Res	Type
4	B	31	U
4	B	38	A
4	B	41	A
4	B	42	G
4	B	48	C
4	B	66	C
4	B	68	A
4	B	83	C
4	B	98	A
4	B	103	C
4	B	117	U
4	B	118	U

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	B	0	G
4	B	2	G
4	B	3	A
4	B	15	U
4	B	16	U
4	B	29	C
4	B	30	G
4	B	65	C
4	B	82	U
4	B	97	U

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 26 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

### 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	E	28/29 (96%)	-0.61	0	100	100	10, 25, 63, 76	0
2	H	11/12 (91%)	-0.28	0	100	100	21, 26, 78, 82	0
3	Z	982/1108 (88%)	-0.03	30 (3%)	49	48	9, 39, 87, 140	0
4	B	115/123 (93%)	-0.26	4 (3%)	44	43	13, 40, 71, 90	0
All	All	1136/1272 (89%)	-0.07	34 (2%)	50	49	9, 39, 85, 140	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	997	ILE	5.7
3	Z	208	ARG	4.5
4	B	90	G	4.4
3	Z	662	ILE	4.3
3	Z	308	GLU	4.2
3	Z	678	ASN	4.1
3	Z	674	SER	3.7
3	Z	594	ASP	3.5
3	Z	526	SER	3.4
3	Z	692	ILE	3.1
3	Z	341	LYS	3.0
3	Z	321	ASP	2.9
3	Z	307	ASP	2.9
3	Z	1006	PHE	2.9
3	Z	194	ASN	2.9
3	Z	664	GLU	2.7
3	Z	658	GLN	2.7
3	Z	670	THR	2.7
3	Z	649	PHE	2.6
3	Z	370	ASP	2.4
3	Z	668	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
3	Z	690	ILE	2.3
3	Z	278	ARG	2.3
3	Z	525	LYS	2.3
3	Z	694	GLU	2.3
3	Z	1043	ASP	2.2
3	Z	665	ARG	2.2
4	B	85	C	2.2
4	B	53	G	2.1
3	Z	138	SER	2.1
3	Z	302	LYS	2.1
4	B	57	G	2.1
3	Z	283	THR	2.1
3	Z	150	ALA	2.1

## 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 monosaccharides 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( $\text{\AA}^2$ )	Q<0.9
5	MG	B	211	1/1	0.42	0.60	49,49,49,49	0
5	MG	E	101	1/1	0.48	0.16	23,23,23,23	0
5	MG	Z	1201	1/1	0.59	0.25	44,44,44,44	0
5	MG	B	216	1/1	0.59	0.26	40,40,40,40	0
5	MG	B	210	1/1	0.64	0.41	41,41,41,41	0
5	MG	Z	1205	1/1	0.67	0.41	54,54,54,54	0
5	MG	B	203	1/1	0.68	0.35	36,36,36,36	0
5	MG	B	202	1/1	0.70	0.47	46,46,46,46	0
5	MG	Z	1202	1/1	0.71	0.47	40,40,40,40	0
5	MG	B	208	1/1	0.76	0.40	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	Z	1203	1/1	0.82	0.55	30,30,30,30	0
5	MG	B	206	1/1	0.83	0.27	28,28,28,28	0
5	MG	B	213	1/1	0.83	0.21	28,28,28,28	0
5	MG	B	215	1/1	0.83	0.27	27,27,27,27	0
5	MG	B	207	1/1	0.83	0.44	55,55,55,55	0
5	MG	B	218	1/1	0.83	0.23	41,41,41,41	0
5	MG	B	214	1/1	0.84	0.20	25,25,25,25	0
5	MG	Z	1204	1/1	0.85	0.41	46,46,46,46	0
5	MG	B	204	1/1	0.85	0.46	36,36,36,36	0
5	MG	B	212	1/1	0.86	0.15	20,20,20,20	0
5	MG	B	209	1/1	0.86	0.52	44,44,44,44	0
5	MG	H	101	1/1	0.87	0.34	32,32,32,32	0
5	MG	B	217	1/1	0.88	0.51	43,43,43,43	0
5	MG	B	205	1/1	0.91	0.16	32,32,32,32	0
5	MG	B	201	1/1	0.91	0.56	41,41,41,41	0
5	MG	B	219	1/1	0.91	0.16	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.