



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:57 PM UTC

PDB ID : 5WTI / pdb_00005wti
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

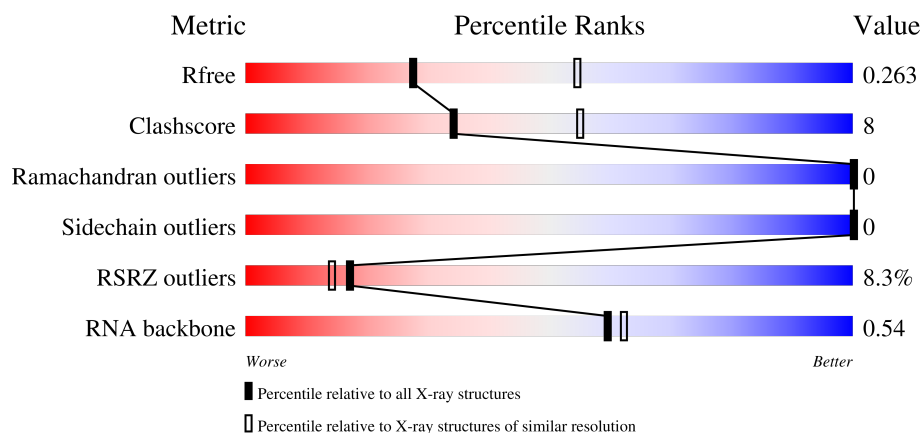
1 Overall quality at a glance

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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)
RNA backbone	3983	1075 (2.90-2.46)

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 ≥ 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	8% 66% 31% .
2	H	12	8% 75% 17% 8%
3	Z	1108	8% 71% 17% 11%
4	B	123	5% 54% 25% 15% 7%

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	201	-	-	-	X
5	MG	B	202	-	-	-	X
5	MG	B	207	-	-	-	X
5	MG	B	208	-	-	-	X
5	MG	B	209	-	-	-	X
5	MG	B	211	-	-	-	X

2 Entry composition [i](#)

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 (CCD ID: 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

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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) 89.2 (19.91-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.67Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.217 , 0.264 0.216 , 0.263	Depositor DCC
R_{free} test set	2000 reflections (3.59%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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 [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	0.26	0/633	0.40	0/972
2	H	0.27	0/253	0.47	0/389
3	Z	0.23	0/8058	0.41	1/10857 (0.0%)
4	B	0.16	0/2751	0.38	0/4281
All	All	0.22	0/11695	0.40	1/16499 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	254	ARG	CB-CG-CD	5.16	123.18	111.30

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
2	H	227	0	126	2	0
3	Z	7888	0	7706	126	0
4	B	2462	0	1240	37	0
5	B	19	0	0	0	0
5	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	154	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 8.

All (154) 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	1.74	0.69
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:34:TYR:HE2	3:Z:219:MET:HE3	1.70	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:612:HIS:NE2	3:Z:615:SER:OG	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:190:PHE:HB3	3:Z:219:MET:HE1	1.96	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:896:THR:C	3:Z:898:GLU:H	2.25	0.45
3:Z:1054:GLU:O	3:Z:1055:LYS:HG2	2.17	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:320:LYS:HZ2	4:B:121:U:HO3'	1.56	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
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:615:SER:O	4:B:18:G:O2'	2.33	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
3:Z:194:ASN:CG	3:Z:194:ASN:O	2.64	0.40
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
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%)	815 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	Z	24	HIS
3	Z	36	ASN
3	Z	56	ASN
3	Z	210	GLN
3	Z	267	GLN
3	Z	273	GLN
3	Z	453	GLN
3	Z	724	HIS

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
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

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Mol	Chain	Res	Type
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 oligosaccharides 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 ⓘ

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, 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	E	28/29 (96%)	-0.34	0 100 100	10, 25, 63, 76	0
2	H	11/12 (91%)	0.25	1 (9%) 15 12	21, 26, 78, 82	0
3	Z	982/1108 (88%)	0.34	87 (8%) 15 13	9, 39, 87, 140	0
4	B	115/123 (93%)	0.14	6 (5%) 33 28	13, 40, 71, 90	0
All	All	1136/1272 (89%)	0.31	94 (8%) 17 14	9, 39, 85, 140	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	658	GLN	5.1
3	Z	672	TRP	4.3
3	Z	308	GLU	4.2
3	Z	977	ALA	4.1
4	B	54	U	4.0
3	Z	661	ASP	3.8
3	Z	138	SER	3.6
3	Z	673	ILE	3.6
3	Z	678	ASN	3.6
3	Z	1004	GLY	3.6
3	Z	901	GLN	3.6
3	Z	697	TYR	3.5
3	Z	649	PHE	3.5
3	Z	208	ARG	3.4
3	Z	696	MET	3.4
3	Z	194	ASN	3.3
3	Z	1045	PHE	3.3
3	Z	975	CYS	3.2
3	Z	150	ALA	3.2
3	Z	1044	SER	3.2
3	Z	291	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
3	Z	703	TRP	3.1
3	Z	351	HIS	3.1
3	Z	715	GLU	3.1
3	Z	676	GLN	3.1
3	Z	1005	TYR	3.0
3	Z	662	ILE	3.0
3	Z	677	GLU	3.0
3	Z	199	LYS	3.0
3	Z	665	ARG	2.9
3	Z	762	THR	2.9
3	Z	341	LYS	2.9
3	Z	257	GLU	2.8
3	Z	254	ARG	2.8
3	Z	997	ILE	2.8
3	Z	1085	ILE	2.8
4	B	2	G	2.8
3	Z	1006	PHE	2.8
3	Z	675	ARG	2.8
3	Z	1056	LEU	2.8
3	Z	321	ASP	2.8
3	Z	83	THR	2.8
3	Z	248	HIS	2.7
3	Z	1007	ILE	2.7
3	Z	307	ASP	2.7
3	Z	833	TYR	2.7
3	Z	899	LYS	2.7
3	Z	900	LEU	2.6
3	Z	1070	ASP	2.6
3	Z	315	TYR	2.6
3	Z	664	GLU	2.6
3	Z	694	GLU	2.6
3	Z	326	HIS	2.6
3	Z	699	PRO	2.6
4	B	53	G	2.5
3	Z	526	SER	2.5
3	Z	1071	LYS	2.5
3	Z	695	LEU	2.5
3	Z	1052	LYS	2.5
3	Z	693	ARG	2.5
3	Z	295	GLY	2.5
3	Z	306	MET	2.5
4	B	66	C	2.4

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Mol	Chain	Res	Type	RSRZ
3	Z	663	THR	2.4
3	Z	689	LEU	2.4
3	Z	700	TYR	2.3
4	B	1	C	2.3
3	Z	1069	SER	2.3
3	Z	316	LEU	2.3
3	Z	356	TYR	2.3
3	Z	713	ARG	2.3
3	Z	692	ILE	2.3
3	Z	525	LYS	2.3
3	Z	698	LYS	2.3
3	Z	353	GLU	2.3
3	Z	340	SER	2.3
3	Z	702	ASP	2.3
3	Z	1010	ASP	2.2
3	Z	1002	GLY	2.2
3	Z	298	GLU	2.2
3	Z	668	ARG	2.2
3	Z	283	THR	2.1
3	Z	927	ASP	2.1
3	Z	970	PHE	2.1
3	Z	999	GLU	2.1
3	Z	1084	ARG	2.1
3	Z	639	ASN	2.1
3	Z	836	TYR	2.1
3	Z	774	GLN	2.1
3	Z	293	LEU	2.1
2	H	1	DG	2.0
3	Z	670	THR	2.0
3	Z	357	LEU	2.0
4	B	84	U	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
5	MG	B	216	1/1	0.49	0.24	40,40,40,40	0
5	MG	B	209	1/1	0.52	0.56	44,44,44,44	0
5	MG	Z	1201	1/1	0.52	0.29	44,44,44,44	0
5	MG	B	214	1/1	0.54	0.17	25,25,25,25	0
5	MG	B	202	1/1	0.56	0.43	46,46,46,46	0
5	MG	B	212	1/1	0.56	0.12	20,20,20,20	0
5	MG	B	203	1/1	0.56	0.27	36,36,36,36	0
5	MG	B	207	1/1	0.56	0.43	55,55,55,55	0
5	MG	Z	1205	1/1	0.61	0.35	54,54,54,54	0
5	MG	E	101	1/1	0.63	0.12	23,23,23,23	0
5	MG	Z	1204	1/1	0.64	0.21	46,46,46,46	0
5	MG	H	101	1/1	0.65	0.28	32,32,32,32	0
5	MG	B	211	1/1	0.66	0.47	49,49,49,49	0
5	MG	Z	1202	1/1	0.66	0.34	40,40,40,40	0
5	MG	B	218	1/1	0.69	0.28	41,41,41,41	0
5	MG	B	213	1/1	0.72	0.14	28,28,28,28	0
5	MG	B	208	1/1	0.72	0.41	58,58,58,58	0
5	MG	B	201	1/1	0.74	0.44	41,41,41,41	0
5	MG	B	205	1/1	0.75	0.22	32,32,32,32	0
5	MG	B	215	1/1	0.75	0.27	27,27,27,27	0
5	MG	Z	1203	1/1	0.76	0.38	30,30,30,30	0
5	MG	B	206	1/1	0.79	0.14	28,28,28,28	0
5	MG	B	210	1/1	0.80	0.41	41,41,41,41	0
5	MG	B	204	1/1	0.82	0.36	36,36,36,36	0
5	MG	B	217	1/1	0.88	0.46	43,43,43,43	0
5	MG	B	219	1/1	0.89	0.07	28,28,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.