



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:13 PM UTC

PDB ID : 6M0W / pdb_00006m0w
Title : Crystal structure of Streptococcus thermophilus Cas9 in complex with the AGAA PAM
Authors : Zhang, Y.; Zhang, H.; Xu, X.; Wang, Y.; Chen, W.; Wang, Y.; Wu, Z.; Tang, N.; Wang, Y.; Zhao, S.; Gan, J.; Ji, Q.
Deposited on : 2020-02-23
Resolution : 2.76 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

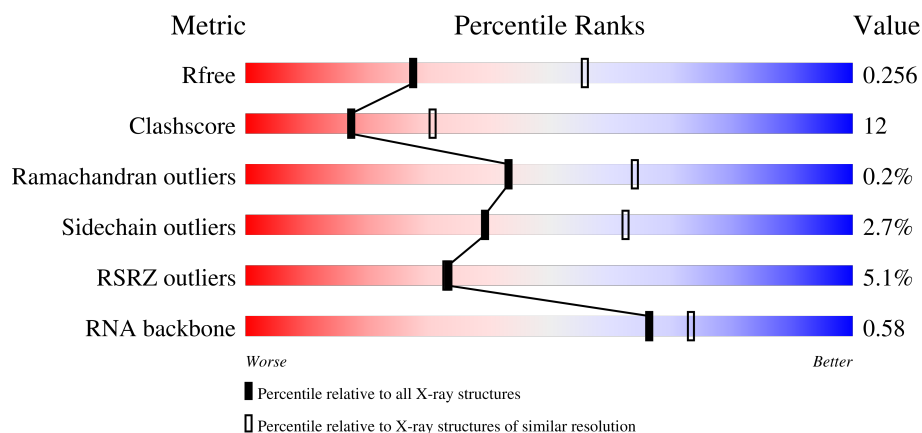
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)
RNA backbone	3983	1179 (3.00-2.52)

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	B	72	
2	C	28	
3	D	8	
4	A	1122	

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	A	1202	-	-	-	X
5	MG	A	1203	-	-	-	X
5	MG	B	101	-	-	-	X
5	MG	D	101	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10518 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 RNA chain called RNA (72-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	72	Total	C	N	O	P	0	0	0
			1520	680	276	493	71			

- Molecule 2 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	28	Total	C	N	O	P	0	0	0
			562	273	90	172	27			

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*AP*AP*GP*AP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	8	Total	C	N	O	P	0	0	0
			165	79	38	41	7			

- Molecule 4 is a protein called CRISPR-associated endonuclease Cas9 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1032	Total	C	N	O	S	0	0	0
			8247	5223	1435	1572	17			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q03LF7
A	1	GLY	-	expression tag	UNP Q03LF7
A	599	ALA	HIS	engineered mutation	UNP Q03LF7

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Mg 1	0	0
5	D	1	Total 1	Mg 1	0	0
5	A	3	Total 3	Mg 3	0	0

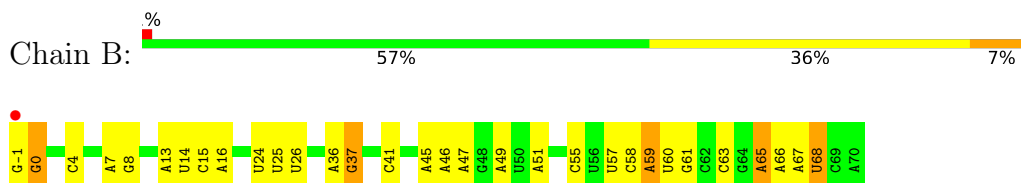
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total 4	O 4	0	0
6	C	2	Total 2	O 2	0	0
6	A	13	Total 13	O 13	0	0

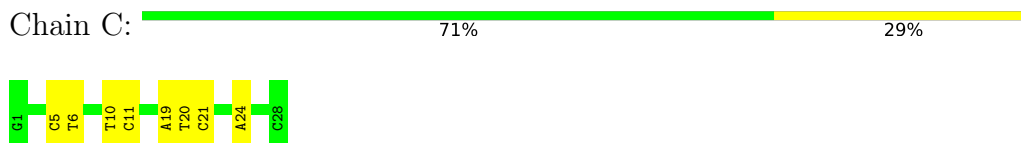
3 Residue-property plots [i](#)

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.

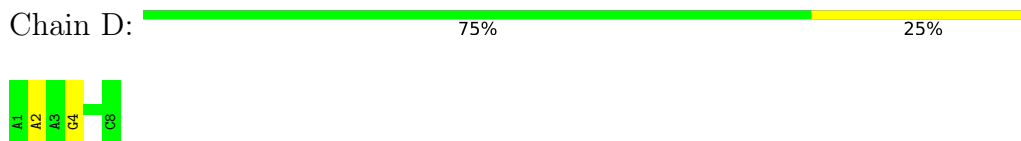
- Molecule 1: RNA (72-MER)



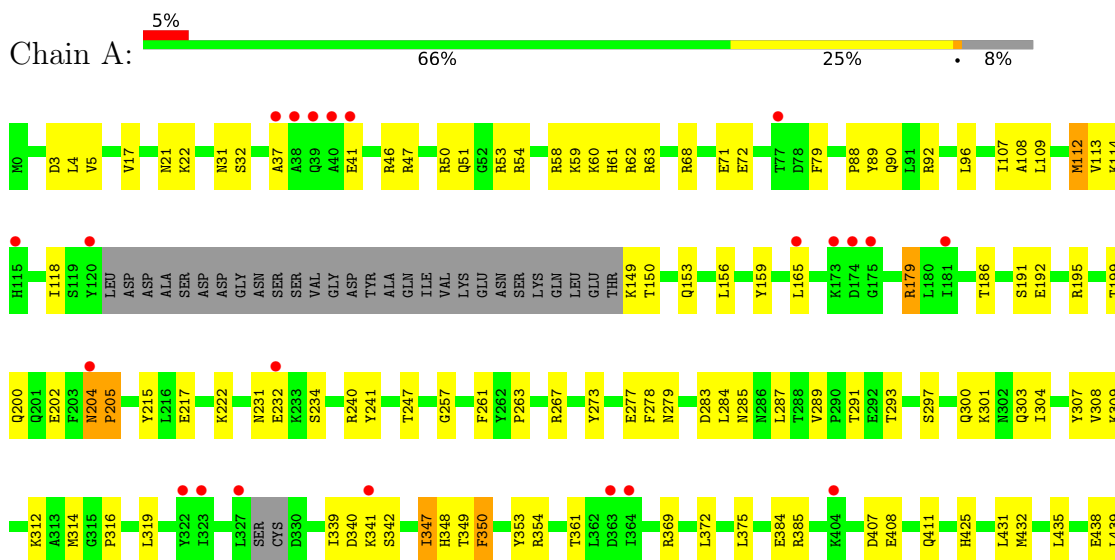
- Molecule 2: DNA (28-MER)

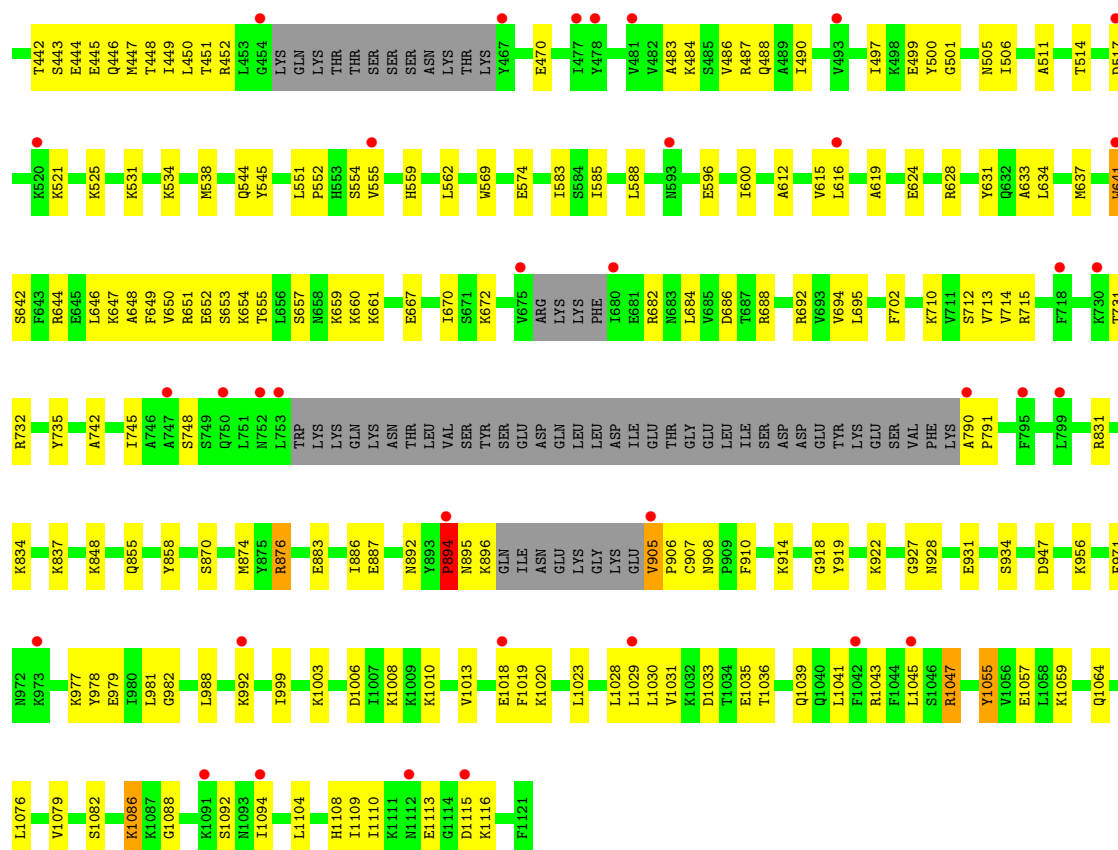


- Molecule 3: DNA (5'-D(*AP*AP*AP*GP*AP*AP*GP*C)-3')



- Molecule 4: CRISPR-associated endonuclease Cas9 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	321.71 Å 75.33 Å 70.30 Å 90.00° 93.47° 90.00°	Depositor
Resolution (Å)	48.87 – 2.76 48.87 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.87-2.76) 99.2 (48.87-2.76)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.77 Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.220 , 0.260 0.221 , 0.256	Depositor DCC
R_{free} test set	2202 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.5	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	0.93	EDS
Total number of atoms	10518	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: 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	0.26	0/1702	0.37	0/2652
2	C	0.41	0/626	0.59	0/963
3	D	0.54	0/187	0.58	0/287
4	A	0.49	0/8391	0.59	11/11301 (0.1%)
All	All	0.46	0/10906	0.56	11/15203 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	928	ASN	N-CA-C	7.38	121.55	112.54
4	A	1047	ARG	N-CA-C	-6.11	98.77	108.73
4	A	517	ASP	N-CA-C	5.94	117.76	111.28
4	A	204	ASN	CA-C-N	-5.72	114.35	120.47
4	A	204	ASN	C-N-CA	-5.72	114.35	120.47
4	A	927	GLY	CA-C-N	5.32	129.60	120.72
4	A	927	GLY	C-N-CA	5.32	129.60	120.72
4	A	905	VAL	CA-C-N	-5.32	114.77	120.03
4	A	905	VAL	C-N-CA	-5.32	114.77	120.03
4	A	892	ASN	N-CA-C	5.19	119.30	112.92
4	A	894	PRO	N-CA-C	5.05	122.88	112.47

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	1520	0	763	31	0
2	C	562	0	322	7	0
3	D	165	0	90	2	0
4	A	8247	0	8128	234	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	13	0	0	1	0
6	B	4	0	0	0	0
6	C	2	0	0	0	0
All	All	10518	0	9303	247	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 12.

All (247) 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)
4:A:896:LYS:N	4:A:907:CYS:SG	2.40	0.94
4:A:1109:ILE:C	4:A:1110:ILE:HD12	1.92	0.93
4:A:309:LYS:HG3	4:A:353:TYR:HE2	1.34	0.90
4:A:273:TYR:HB2	4:A:372:LEU:HD23	1.54	0.90
4:A:1115:ASP:OD2	4:A:1116:LYS:NZ	2.06	0.88
4:A:17:VAL:HB	4:A:31:ASN:HB3	1.56	0.87
4:A:858:TYR:HB2	4:A:908:ASN:ND2	1.93	0.84
4:A:309:LYS:HG3	4:A:353:TYR:CE2	2.15	0.81
4:A:1010:LYS:H	4:A:1010:LYS:HD2	1.48	0.78
4:A:971:PHE:HB3	4:A:1018:GLU:OE2	1.84	0.77
4:A:1108:HIS:O	4:A:1110:ILE:CD1	2.33	0.77
4:A:1010:LYS:HD2	4:A:1010:LYS:N	1.98	0.77
4:A:552:PRO:O	4:A:555:VAL:HG22	1.85	0.75
4:A:53:ARG:NH1	6:A:1301:HOH:O	2.20	0.74
4:A:159:TYR:HB2	4:A:165:LEU:HD21	1.71	0.73
4:A:1028:LEU:HD23	4:A:1043:ARG:HB3	1.73	0.71
4:A:855:GLN:HE22	4:A:906:PRO:HB2	1.56	0.70
4:A:446:GLN:O	4:A:450:LEU:HD12	1.92	0.69
4:A:1110:ILE:HD12	4:A:1110:ILE:N	2.08	0.69
4:A:874:MET:HE1	4:A:886:ILE:HG13	1.72	0.69
4:A:1033:ASP:OD1	4:A:1035:GLU:HG2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:634:LEU:HA	4:A:637:MET:HE3	1.75	0.69
4:A:240:ARG:NH2	4:A:241:TYR:OH	2.26	0.68
1:B:63:C:OP2	4:A:54:ARG:NH1	2.27	0.68
4:A:46:ARG:HD3	4:A:50:ARG:HH21	1.59	0.68
4:A:834:LYS:O	4:A:876:ARG:NH1	2.26	0.68
1:B:63:C:P	4:A:54:ARG:NH1	2.67	0.67
4:A:277:GLU:OE1	4:A:369:ARG:NH1	2.29	0.66
4:A:442:THR:HG21	4:A:452:ARG:HH22	1.60	0.66
4:A:585:ILE:HA	4:A:588:LEU:HB3	1.79	0.65
4:A:316:PRO:HB3	4:A:347:ILE:HG22	1.78	0.65
4:A:447:MET:HE2	4:A:451:THR:HG23	1.80	0.63
4:A:484:LYS:HA	4:A:487:ARG:NH1	2.14	0.63
4:A:641:TRP:HH2	4:A:649:PHE:HD2	1.47	0.62
4:A:347:ILE:HG13	4:A:348:HIS:N	2.14	0.62
4:A:1108:HIS:O	4:A:1110:ILE:HD12	1.99	0.62
4:A:291:THR:HG23	4:A:293:THR:H	1.64	0.61
4:A:1018:GLU:CD	4:A:1018:GLU:H	2.08	0.61
4:A:279:ASN:HB3	4:A:348:HIS:CE1	2.35	0.61
4:A:3:ASP:HA	4:A:22:LYS:HD3	1.82	0.61
4:A:303:GLN:O	4:A:307:TYR:N	2.32	0.61
4:A:444:GLU:OE2	4:A:452:ARG:NH2	2.20	0.61
4:A:919:TYR:HB2	4:A:931:GLU:HG2	1.82	0.60
4:A:407:ASP:O	4:A:411:GLN:HG2	2.00	0.60
4:A:1109:ILE:N	4:A:1109:ILE:HD12	2.18	0.59
1:B:15:C:OP1	4:A:54:ARG:NH2	2.35	0.59
4:A:858:TYR:CB	4:A:908:ASN:ND2	2.64	0.59
4:A:312:LYS:O	4:A:354:ARG:NH1	2.36	0.59
1:B:-1:G:H2'	1:B:0:G:C8	2.38	0.59
1:B:63:C:OP1	4:A:54:ARG:NH1	2.34	0.59
2:C:24:DA:H2''	4:A:339:ILE:CG2	2.33	0.58
4:A:855:GLN:NE2	4:A:906:PRO:HG2	2.19	0.58
4:A:308:VAL:HG12	4:A:314:MET:HE2	1.86	0.58
4:A:1018:GLU:OE1	4:A:1018:GLU:N	2.35	0.58
1:B:60:U:O4	4:A:240:ARG:NH2	2.37	0.57
4:A:506:ILE:HD12	4:A:702:PHE:HE2	1.68	0.57
4:A:648:ALA:O	4:A:652:GLU:HG3	2.05	0.57
4:A:682:ARG:NH1	4:A:686:ASP:OD2	2.38	0.57
4:A:894:PRO:O	4:A:895:ASN:HB3	2.04	0.57
4:A:444:GLU:HB3	4:A:448:THR:OG1	2.04	0.57
1:B:13:A:OP2	4:A:47:ARG:NH2	2.38	0.56
3:D:2:DA:H3'	4:A:1045:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:4:LEU:HD23	4:A:21:ASN:HA	1.87	0.56
4:A:914:LYS:HD2	4:A:919:TYR:CE1	2.39	0.56
4:A:204:ASN:OD1	4:A:205:PRO:HD2	2.06	0.56
4:A:569:TRP:CZ2	4:A:574:GLU:HG2	2.40	0.56
4:A:261:PHE:HB2	4:A:431:LEU:HD13	1.87	0.56
4:A:883:GLU:HA	4:A:887:GLU:HG3	1.90	0.54
4:A:31:ASN:HD22	4:A:32:SER:N	2.06	0.54
1:B:63:C:P	4:A:54:ARG:HH12	2.31	0.54
4:A:284:LEU:HA	4:A:287:LEU:HD12	1.89	0.54
4:A:855:GLN:NE2	4:A:906:PRO:HB2	2.22	0.54
4:A:919:TYR:CB	4:A:931:GLU:HG2	2.38	0.53
4:A:982:GLY:HA3	4:A:1047:ARG:HG2	1.88	0.53
4:A:438:GLU:O	4:A:442:THR:HG23	2.07	0.53
4:A:37:ALA:O	4:A:41:GLU:HG3	2.08	0.53
4:A:314:MET:HE3	4:A:319:LEU:HB2	1.90	0.53
4:A:1045:LEU:HD23	4:A:1057:GLU:HG2	1.91	0.53
4:A:231:ASN:HA	4:A:241:TYR:CE2	2.43	0.53
4:A:551:LEU:HD23	4:A:552:PRO:HD2	1.89	0.53
4:A:600:ILE:HD11	4:A:615:VAL:HG13	1.89	0.53
4:A:914:LYS:HD2	4:A:919:TYR:HE1	1.72	0.53
4:A:559:HIS:CD2	4:A:562:LEU:HG	2.43	0.53
1:B:55:C:OP2	4:A:992:LYS:NZ	2.42	0.53
4:A:446:GLN:C	4:A:450:LEU:HD12	2.33	0.53
4:A:855:GLN:NE2	4:A:906:PRO:CG	2.72	0.53
4:A:650:VAL:HG13	4:A:661:LYS:HG2	1.91	0.52
4:A:521:LYS:O	4:A:525:LYS:HG2	2.10	0.52
4:A:1109:ILE:N	4:A:1109:ILE:CD1	2.72	0.52
4:A:848:LYS:HD2	4:A:934:SER:HB3	1.92	0.52
4:A:1030:LEU:HD21	4:A:1039:GLN:NE2	2.24	0.52
4:A:647:LYS:HE2	4:A:651:ARG:HH21	1.74	0.52
4:A:545:TYR:HB2	4:A:585:ILE:HD12	1.91	0.52
4:A:646:LEU:CD1	4:A:650:VAL:HG23	2.40	0.52
4:A:1035:GLU:HG3	4:A:1036:THR:H	1.75	0.52
4:A:445:GLU:O	4:A:449:ILE:HG13	2.10	0.51
4:A:47:ARG:O	4:A:51:GLN:HG3	2.10	0.51
4:A:497:ILE:O	4:A:501:GLY:N	2.42	0.51
4:A:31:ASN:HD22	4:A:32:SER:H	1.58	0.51
2:C:20:DT:H2'	2:C:21:DC:C6	2.46	0.51
4:A:670:ILE:O	4:A:670:ILE:HG13	2.10	0.51
4:A:445:GLU:OE2	4:A:448:THR:HG23	2.11	0.51
4:A:552:PRO:O	4:A:555:VAL:CG2	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:A:O2'	4:A:61:HIS:HE1	1.94	0.50
4:A:484:LYS:O	4:A:488:GLN:HG2	2.12	0.50
4:A:695:LEU:HD11	4:A:713:VAL:CG2	2.41	0.50
4:A:895:ASN:C	4:A:907:CYS:SG	2.94	0.49
4:A:1010:LYS:H	4:A:1010:LYS:CD	2.21	0.49
4:A:1055:TYR:HA	4:A:1088:GLY:HA2	1.94	0.49
2:C:5:DC:H2''	2:C:6:DT:H72	1.94	0.49
1:B:49:A:OP2	4:A:63:ARG:NH2	2.45	0.49
4:A:68:ARG:O	4:A:72:GLU:HG3	2.11	0.49
4:A:435:LEU:O	4:A:439:LEU:HD12	2.12	0.49
4:A:947:ASP:OD2	4:A:956:LYS:HD2	2.13	0.49
4:A:54:ARG:O	4:A:58:ARG:HG3	2.12	0.49
4:A:979:GLU:HB3	4:A:1013:VAL:HG22	1.95	0.48
4:A:3:ASP:O	4:A:22:LYS:HG2	2.13	0.48
2:C:24:DA:H2''	4:A:339:ILE:HG22	1.94	0.48
4:A:914:LYS:HA	4:A:918:GLY:O	2.14	0.48
4:A:596:GLU:HG3	4:A:619:ALA:HA	1.95	0.48
4:A:361:THR:OG1	4:A:408:GLU:OE1	2.25	0.48
4:A:1029:LEU:O	4:A:1041:LEU:HD12	2.13	0.48
4:A:90:GLN:HA	4:A:156:LEU:HD22	1.96	0.48
4:A:1110:ILE:CD1	4:A:1110:ILE:N	2.76	0.48
4:A:837:LYS:O	4:A:837:LYS:HD3	2.14	0.47
4:A:977:LYS:HG2	4:A:1092:SER:HA	1.96	0.47
4:A:646:LEU:HD12	4:A:650:VAL:HG23	1.96	0.47
4:A:384:GLU:HG2	4:A:385:ARG:H	1.79	0.47
4:A:858:TYR:HB2	4:A:908:ASN:HD21	1.77	0.47
4:A:1031:VAL:HG11	4:A:1076:LEU:HD11	1.96	0.47
1:B:55:C:P	4:A:992:LYS:NZ	2.88	0.47
4:A:484:LYS:HA	4:A:487:ARG:HH11	1.80	0.47
4:A:583:ILE:HD13	4:A:616:LEU:HD12	1.96	0.47
4:A:62:ARG:HB3	4:A:113:VAL:HG13	1.96	0.47
4:A:544:GLN:HB2	4:A:585:ILE:HD11	1.96	0.47
4:A:855:GLN:HE21	4:A:906:PRO:HG2	1.78	0.47
4:A:88:PRO:HB3	4:A:107:ILE:HG22	1.97	0.47
4:A:285:ASN:OD1	4:A:443:SER:HA	2.15	0.47
4:A:545:TYR:HB3	4:A:551:LEU:HD21	1.97	0.47
4:A:731:THR:OG1	4:A:732:ARG:N	2.48	0.47
4:A:149:LYS:HG2	4:A:153:GLN:OE1	2.15	0.46
4:A:257:GLY:O	4:A:267:ARG:HG3	2.15	0.46
1:B:4:C:Cl'	4:A:446:GLN:HE21	2.27	0.46
1:B:4:C:Cl'	4:A:446:GLN:NE2	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:179:ARG:NH1	4:A:624:GLU:HB2	2.30	0.46
4:A:5:VAL:HG23	4:A:505:ASN:HB3	1.97	0.46
4:A:445:GLU:OE2	4:A:447:MET:HB3	2.16	0.46
4:A:483:ALA:O	4:A:487:ARG:HG3	2.16	0.46
4:A:905:VAL:HG12	4:A:905:VAL:O	2.15	0.46
4:A:347:ILE:HG13	4:A:348:HIS:H	1.80	0.46
4:A:642:SER:OG	4:A:644:ARG:HG2	2.16	0.46
4:A:60:LYS:O	4:A:63:ARG:HG2	2.15	0.46
4:A:350:PHE:O	4:A:354:ARG:HG3	2.16	0.46
4:A:1035:GLU:HG3	4:A:1036:THR:N	2.31	0.46
4:A:514:THR:HG22	4:A:715:ARG:NH1	2.31	0.45
4:A:534:LYS:O	4:A:538:MET:HG2	2.16	0.45
4:A:988:LEU:CD2	4:A:999:ILE:HB	2.47	0.45
4:A:195:ARG:O	4:A:199:THR:HG23	2.16	0.45
4:A:200:GLN:O	4:A:204:ASN:N	2.39	0.45
4:A:714:VAL:HG21	4:A:748:SER:OG	2.15	0.45
4:A:742:ALA:HA	4:A:745:ILE:HD12	1.99	0.45
4:A:870:SER:O	4:A:876:ARG:NH2	2.48	0.45
1:B:65:A:H3'	4:A:46:ARG:HG3	1.98	0.45
3:D:4:DG:O6	4:A:1086:LYS:NZ	2.44	0.45
4:A:109:LEU:HB3	4:A:215:TYR:CE1	2.52	0.45
4:A:150:THR:HB	4:A:192:GLU:HB2	1.98	0.45
1:B:8:G:OP1	4:A:534:LYS:NZ	2.39	0.45
4:A:278:PHE:HB3	4:A:432:MET:HE2	1.98	0.45
4:A:855:GLN:HE22	4:A:906:PRO:CB	2.26	0.45
4:A:112:MET:HE2	4:A:112:MET:HB2	1.79	0.44
1:B:4:C:H1'	4:A:446:GLN:HE21	1.82	0.44
1:B:24:U:H2'	1:B:25:U:C6	2.53	0.44
4:A:4:LEU:CD2	4:A:21:ASN:HA	2.47	0.44
4:A:631:TYR:CD2	4:A:667:GLU:HA	2.53	0.44
4:A:261:PHE:O	4:A:263:PRO:HD3	2.17	0.44
4:A:283:ASP:HB3	4:A:347:ILE:CD1	2.48	0.44
4:A:486:VAL:HG22	4:A:694:VAL:HG23	1.99	0.44
4:A:654:LYS:HE2	4:A:654:LYS:HB2	1.75	0.44
4:A:790:ALA:HB3	4:A:791:PRO:HD3	1.99	0.44
4:A:914:LYS:HZ2	4:A:919:TYR:HE1	1.64	0.44
4:A:988:LEU:HD23	4:A:999:ILE:HB	1.99	0.44
2:C:24:DA:H2''	4:A:339:ILE:HG21	1.99	0.44
4:A:855:GLN:HE21	4:A:906:PRO:CG	2.30	0.44
4:A:1108:HIS:O	4:A:1110:ILE:HD11	2.14	0.44
1:B:16:A:O2'	4:A:222:LYS:HE3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:19:DA:H2'	2:C:20:DT:C6	2.52	0.44
4:A:657:SER:O	4:A:661:LYS:HG3	2.18	0.43
4:A:4:LEU:HD21	4:A:21:ASN:OD1	2.18	0.43
1:B:36:A:N7	1:B:37:G:H1'	2.34	0.43
4:A:118:ILE:O	4:A:186:THR:OG1	2.32	0.43
4:A:735:TYR:OH	4:A:1064:GLN:HB2	2.18	0.43
4:A:283:ASP:HB3	4:A:347:ILE:HD12	2.00	0.43
4:A:4:LEU:HD21	4:A:21:ASN:CG	2.44	0.43
4:A:505:ASN:HA	4:A:710:LYS:O	2.19	0.43
4:A:505:ASN:ND2	4:A:712:SER:OG	2.44	0.43
4:A:628:ARG:HB2	4:A:633:ALA:HB2	2.00	0.43
4:A:978:TYR:HE1	4:A:1020:LYS:HZ2	1.61	0.43
1:B:36:A:C5	1:B:37:G:H1'	2.54	0.43
4:A:300:GLN:O	4:A:304:ILE:HG13	2.18	0.43
4:A:624:GLU:HG2	4:A:637:MET:HG2	2.01	0.42
1:B:13:A:C6	1:B:14:U:C4	3.07	0.42
4:A:499:GLU:HB3	4:A:500:TYR:CD1	2.53	0.42
4:A:31:ASN:OD1	4:A:1104:LEU:HA	2.19	0.42
1:B:7:A:N3	4:A:341:LYS:NZ	2.64	0.42
1:B:47:A:P	4:A:114:LYS:HZ2	2.38	0.42
4:A:349:THR:O	4:A:350:PHE:HB2	2.19	0.42
4:A:684:LEU:O	4:A:688:ARG:HG3	2.20	0.42
4:A:1003:LYS:O	4:A:1006:ASP:HB2	2.19	0.42
4:A:1110:ILE:O	4:A:1110:ILE:HG22	2.20	0.42
1:B:66:A:H2'	1:B:67:A:O4'	2.19	0.42
4:A:267:ARG:HD3	4:A:425:HIS:O	2.19	0.42
4:A:349:THR:O	4:A:349:THR:CG2	2.68	0.42
4:A:470:GLU:HB3	4:A:490:ILE:HG21	2.01	0.42
4:A:999:ILE:HD11	4:A:1003:LYS:HG2	2.01	0.42
4:A:279:ASN:HB3	4:A:348:HIS:ND1	2.34	0.42
1:B:41:C:OP2	4:A:831:ARG:NH1	2.52	0.42
4:A:59:LYS:HB2	4:A:59:LYS:HE2	1.84	0.42
4:A:914:LYS:NZ	4:A:919:TYR:HE1	2.18	0.42
4:A:1020:LYS:O	4:A:1113:GLU:HB2	2.19	0.41
4:A:92:ARG:HG3	4:A:108:ALA:HB1	2.02	0.41
1:B:68:U:H5''	1:B:68:U:H6	1.84	0.41
4:A:612:ALA:HB3	4:A:659:LYS:HE2	2.02	0.41
4:A:908:ASN:OD1	4:A:910:PHE:N	2.53	0.41
4:A:1023:LEU:HD22	4:A:1029:LEU:HD21	2.02	0.41
4:A:62:ARG:HB3	4:A:113:VAL:CG1	2.50	0.41
4:A:506:ILE:HD12	4:A:702:PHE:CE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:511:ALA:HB3	4:A:688:ARG:HG2	2.02	0.41
4:A:981:LEU:HD12	4:A:1008:LYS:HA	2.03	0.41
4:A:289:VAL:HG23	4:A:291:THR:HG22	2.02	0.41
4:A:660:LYS:HE3	4:A:660:LYS:HB2	1.95	0.41
4:A:855:GLN:NE2	4:A:906:PRO:CB	2.83	0.41
4:A:1018:GLU:CD	4:A:1018:GLU:N	2.75	0.41
4:A:96:LEU:O	4:A:199:THR:HG21	2.21	0.41
4:A:340:ASP:OD1	4:A:342:SER:N	2.47	0.41
4:A:1019:PHE:CG	4:A:1020:LYS:N	2.86	0.41
4:A:71:GLU:HG2	4:A:79:PHE:HE1	1.86	0.40
4:A:267:ARG:HB3	4:A:425:HIS:O	2.21	0.40
1:B:41:C:O2	4:A:922:LYS:NZ	2.48	0.40
1:B:46:A:OP1	4:A:89:TYR:OH	2.26	0.40
2:C:10:DT:H2'	2:C:11:DC:C6	2.56	0.40
4:A:297:SER:O	4:A:301:LYS:HE3	2.21	0.40
4:A:634:LEU:HA	4:A:634:LEU:HD23	1.91	0.40
1:B:25:U:H2'	1:B:26:U:C6	2.56	0.40
4:A:384:GLU:HG2	4:A:385:ARG:N	2.36	0.40
4:A:531:LYS:HA	4:A:534:LYS:HD3	2.02	0.40
4:A:895:ASN:O	4:A:896:LYS:CB	2.69	0.40
1:B:45:A:H2'	1:B:46:A:C8	2.57	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
4	A	1018/1122 (91%)	961 (94%)	55 (5%)	2 (0%)	43 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	641	TRP
4	A	894	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	
4	A	875/1000 (88%)	851 (97%)	24 (3%)	39	62

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	112	MET
4	A	179	ARG
4	A	191	SER
4	A	202	GLU
4	A	205	PRO
4	A	217	GLU
4	A	232	GLU
4	A	234	SER
4	A	247	THR
4	A	347	ILE
4	A	350	PHE
4	A	375	LEU
4	A	554	SER
4	A	653	SER
4	A	655	THR
4	A	672	LYS
4	A	692	ARG
4	A	876	ARG
4	A	1055	TYR
4	A	1059	LYS
4	A	1079	VAL
4	A	1082	SER
4	A	1086	LYS
4	A	1094	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	31	ASN
4	A	39	GLN
4	A	61	HIS
4	A	488	GLN
4	A	524	GLN
4	A	527	GLN
4	A	623	GLN
4	A	855	GLN
4	A	1039	GLN
4	A	1108	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	70/72 (97%)	9 (12%)	0

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	0	G
1	B	37	G
1	B	51	A
1	B	57	U
1	B	58	C
1	B	59	A
1	B	61	G
1	B	65	A
1	B	68	U

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 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

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	B	72/72 (100%)	-0.44	1 (1%) 73 73	38, 50, 74, 144	0
2	C	28/28 (100%)	-0.37	0 100 100	37, 48, 82, 91	0
3	D	8/8 (100%)	-0.52	0 100 100	41, 43, 47, 56	0
4	A	1032/1122 (91%)	0.56	57 (5%) 30 30	37, 66, 105, 150	0
All	All	1140/1230 (92%)	0.47	58 (5%) 33 33	37, 64, 105, 150	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	38	ALA	8.1
4	A	40	ALA	7.9
4	A	232	GLU	5.8
4	A	753	LEU	4.9
4	A	747	ALA	4.4
4	A	454	GLY	4.2
4	A	616	LEU	4.1
4	A	790	ALA	4.0
4	A	675	VAL	3.9
4	A	37	ALA	3.8
4	A	322	TYR	3.7
4	A	39	GLN	3.7
4	A	641	TRP	3.6
4	A	323	ILE	3.4
4	A	363	ASP	3.4
4	A	752	ASN	3.3
4	A	174	ASP	3.3
4	A	364	ILE	3.2
4	A	517	ASP	3.1
4	A	593	ASN	3.0
4	A	120	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
4	A	1042	PHE	3.0
4	A	327	LEU	3.0
4	A	1029	LEU	2.9
4	A	181	ILE	2.9
4	A	165	LEU	2.9
4	A	795	PHE	2.9
4	A	77	THR	2.9
4	A	477	ILE	2.9
4	A	41	GLU	2.8
4	A	204	ASN	2.6
4	A	680	ILE	2.5
4	A	750	GLN	2.5
4	A	1115	ASP	2.5
4	A	175	GLY	2.5
4	A	341	LYS	2.4
4	A	481	VAL	2.3
4	A	1091	LYS	2.3
1	B	-1	G	2.3
4	A	478	TYR	2.3
4	A	1018	GLU	2.3
4	A	1112	ASN	2.3
4	A	493	VAL	2.3
4	A	115	HIS	2.2
4	A	1094	ILE	2.2
4	A	799	LEU	2.2
4	A	467	TYR	2.2
4	A	404	LYS	2.2
4	A	1045	LEU	2.2
4	A	520	LYS	2.1
4	A	973	LYS	2.1
4	A	730	LYS	2.1
4	A	905	VAL	2.1
4	A	718	PHE	2.1
4	A	555	VAL	2.0
4	A	173	LYS	2.0
4	A	992	LYS	2.0
4	A	894	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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 [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, 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($\text{\AA}^2$)	Q<0.9
5	MG	A	1202	1/1	-0.28	0.64	75,75,75,75	0
5	MG	B	101	1/1	-0.26	0.47	89,89,89,89	0
5	MG	A	1203	1/1	0.26	0.60	98,98,98,98	0
5	MG	D	101	1/1	0.37	0.86	78,78,78,78	0
5	MG	A	1201	1/1	0.85	0.23	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.