



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:38 PM UTC

PDB ID : 6WBR / pdb_00006wbr
Title : Crystal structure of AceCas9 bound with guide RNA and DNA with 5'-NNNCC-3' PAM
Authors : Li, H.; Das, A.
Deposited on : 2020-03-27
Resolution : 2.91 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

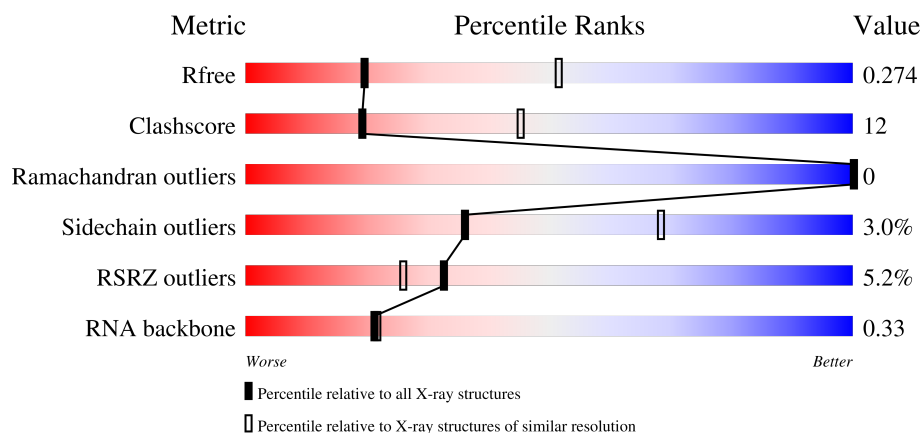
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)
RNA backbone	3983	1016 (3.12-2.72)

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	A	977	5% 71% 25% • •
2	B	94	5% 37% 44% 16% •
3	C	30	33% 67%
4	D	10	100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10160 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 CRISPR-associated endonuclease, Csn1 family, CRISPR-associated endonuclease, Csn1 family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	942	Total	C	N	O	S	0	0	0
			7400	4653	1377	1357	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	518	GLY	-	linker	UNP A0LWB3
A	680	GLY	-	linker	UNP A0LWB3
A	681	GLY	-	linker	UNP A0LWB3
A	682	SER	-	linker	UNP A0LWB3
A	683	ALA	-	linker	UNP A0LWB3
A	684	GLY	-	linker	UNP A0LWB3
A	1135	THR	-	expression tag	UNP A0LWB3
A	1136	ALA	-	expression tag	UNP A0LWB3
A	1137	GLU	-	expression tag	UNP A0LWB3
A	1138	LEU	-	expression tag	UNP A0LWB3

- Molecule 2 is a RNA chain called RNA (94-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	91	Total	C	N	O	P	9	0	0
			1952	866	348	645	93			

- Molecule 3 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	30	Total	C	N	O	P	0	0	0
			606	290	109	178	29			

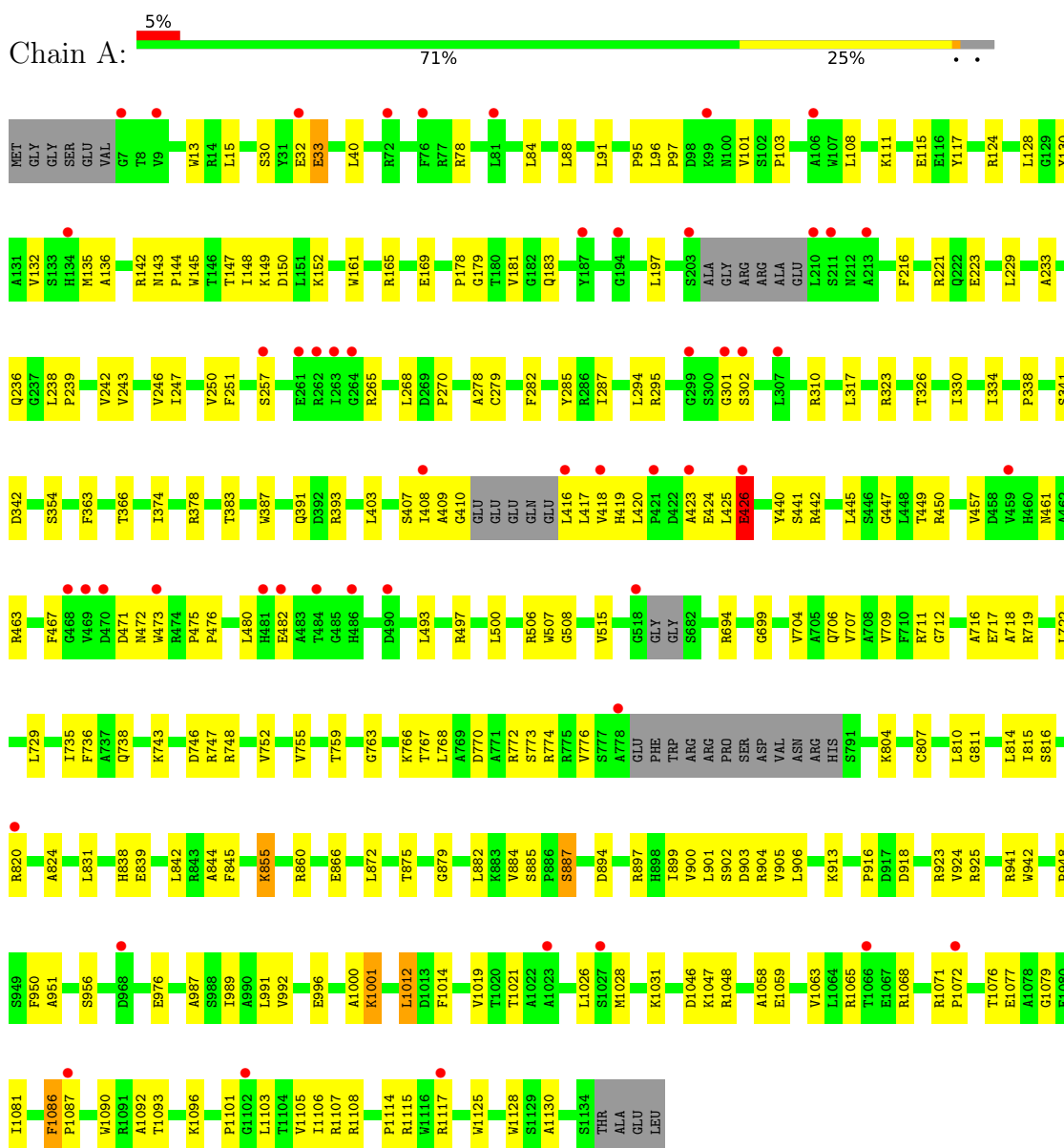
- Molecule 4 is a DNA chain called DNA (5'-D(*AP*TP*AP*CP*CP*TP*GP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			

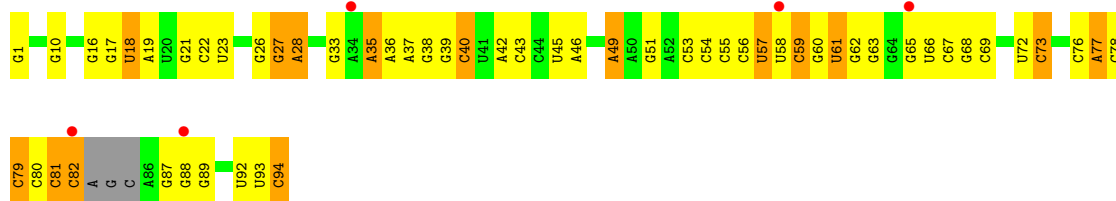
3 Residue-property plots

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.

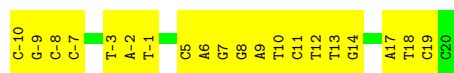
- Molecule 1: CRISPR-associated endonuclease, Csn1 family, CRISPR-associated endonuclease, Csn1 family



- Molecule 2: RNA (94-MER)



- Molecule 3: DNA (30-MER)



- Molecule 4: DNA (5'-D(*AP*TP*AP*CP*CP*TP*GP*GP*CP*G)-3')



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.31Å 119.35Å 177.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.65 – 2.91 74.65 – 2.91	Depositor EDS
% Data completeness (in resolution range)	96.2 (74.65-2.91) 92.5 (74.65-2.91)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.71 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.224 , 0.266 0.230 , 0.274	Depositor DCC
R_{free} test set	1901 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	80.7	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10160	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: GTP

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	0.30	0/7567	0.64	4/10285 (0.0%)
2	B	0.30	0/2144	0.58	0/3338
3	C	0.44	0/678	0.61	0/1043
4	D	0.39	0/226	0.52	0/347
All	All	0.31	0/10615	0.62	4/15013 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	GLU	CA-CB-CG	6.13	126.36	114.10
1	A	1086	PHE	N-CA-C	6.13	122.02	113.57
1	A	425	LEU	CA-C-N	-5.72	111.12	121.14
1	A	425	LEU	C-N-CA	-5.72	111.12	121.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1101	PRO	Peptide
1	A	33	GLU	Peptide

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	A	7400	0	7379	171	1
2	B	1952	0	984	39	1
3	C	606	0	339	21	0
4	D	202	0	114	0	0
All	All	10160	0	8816	221	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 12.

All (221) 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)
2:B:10:G:H1	3:C:11:DC:H5	1.05	0.97
2:B:27:G:H22	2:B:42:A:H61	1.19	0.90
1:A:257:SER:HB2	1:A:409:ALA:HB3	1.62	0.81
3:C:-8:DC:H2''	3:C:-7:DC:H5''	1.65	0.79
1:A:866:GLU:HG2	1:A:901:LEU:HD22	1.67	0.77
1:A:30:SER:HB3	1:A:40:LEU:HD11	1.69	0.75
1:A:135:MET:HE1	1:A:229:LEU:HB2	1.67	0.74
1:A:770:ASP:HB3	1:A:774:ARG:HE	1.55	0.70
1:A:416:LEU:N	1:A:417:LEU:HB3	2.07	0.70
1:A:148:ILE:HD12	1:A:149:LYS:H	1.55	0.70
2:B:17:G:H2'	2:B:18:U:H5'	1.76	0.67
3:C:8:DG:H2'	3:C:9:DA:C8	2.31	0.66
1:A:1076:THR:HG23	1:A:1079:GLY:H	1.60	0.66
2:B:27:G:H22	2:B:42:A:N6	1.92	0.66
1:A:445:LEU:O	1:A:449:THR:HG23	1.95	0.65
3:C:13:DT:H2'	3:C:14:DG:C8	2.31	0.65
1:A:149:LYS:HA	1:A:152:LYS:HD2	1.79	0.65
2:B:76:C:H2'	2:B:77:A:H5'	1.77	0.65
1:A:773:SER:HA	1:A:776:VAL:HG12	1.79	0.65
1:A:148:ILE:HD12	1:A:149:LYS:N	2.11	0.64
1:A:925:ARG:NH1	2:B:49:A:O2'	2.21	0.64
1:A:15:LEU:HD22	1:A:500:LEU:HD13	1.80	0.64
1:A:152:LYS:HE2	1:A:247:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:TRP:CE2	1:A:391:GLN:HG3	2.33	0.63
1:A:755:VAL:HG21	1:A:814:LEU:HD21	1.80	0.63
3:C:8:DG:H2'	3:C:9:DA:H8	1.64	0.63
2:B:17:G:C2'	2:B:18:U:H5'	2.29	0.62
1:A:515:VAL:HB	1:A:709:VAL:HG12	1.80	0.62
2:B:22:C:H2'	2:B:23:U:C6	2.34	0.62
1:A:13:TRP:NE1	1:A:508:GLY:O	2.26	0.62
1:A:717:GLU:HG3	1:A:772:ARG:HB2	1.81	0.62
2:B:27:G:N2	2:B:42:A:H61	1.96	0.62
1:A:719:ARG:HH22	1:A:743:LYS:HD2	1.64	0.62
1:A:763:GLY:O	1:A:766:LYS:HB3	2.00	0.62
1:A:243:VAL:O	1:A:247:ILE:HG23	2.00	0.61
1:A:903:ASP:OD2	1:A:904:ARG:HD3	2.00	0.60
1:A:440:TYR:OH	1:A:463:ARG:NH1	2.34	0.60
2:B:21:G:H2'	2:B:22:C:C6	2.36	0.60
1:A:152:LYS:CE	1:A:247:ILE:HD11	2.32	0.59
2:B:27:G:OP2	2:B:27:G:H8	1.86	0.59
2:B:60:G:N2	2:B:61:U:O4'	2.36	0.58
2:B:81:C:H5''	2:B:81:C:H6	1.66	0.58
1:A:419:HIS:O	1:A:419:HIS:ND1	2.36	0.58
1:A:88:LEU:HD11	1:A:95:PRO:HG3	1.83	0.58
2:B:77:A:H2'	2:B:78:C:H6	1.69	0.58
1:A:989:ILE:HA	1:A:992:VAL:HG22	1.85	0.57
2:B:33:G:C2	2:B:35:A:H5''	2.39	0.57
1:A:887:SER:O	1:A:887:SER:OG	2.23	0.57
1:A:278:ALA:O	1:A:366:THR:HG21	2.04	0.57
1:A:229:LEU:HD23	1:A:247:ILE:HG22	1.87	0.56
3:C:-2:DA:H2''	3:C:-1:DT:H5''	1.88	0.56
1:A:1105:VAL:HG21	1:A:1125:TRP:CE2	2.40	0.56
1:A:124:ARG:HD3	1:A:236:GLN:HG3	1.87	0.55
1:A:417:LEU:HD12	1:A:418:VAL:HG22	1.88	0.54
1:A:882:LEU:HG	1:A:884:VAL:HG22	1.89	0.54
1:A:407:SER:O	1:A:408:ILE:HG13	2.08	0.54
1:A:844:ALA:O	1:A:916:PRO:HG3	2.08	0.54
1:A:473:TRP:CZ3	1:A:475:PRO:HA	2.43	0.54
1:A:441:SER:OG	1:A:442:ARG:N	2.40	0.54
1:A:735:ILE:O	1:A:1076:THR:HG22	2.08	0.54
1:A:842:LEU:HD21	1:A:924:VAL:HG23	1.89	0.54
1:A:763:GLY:O	1:A:767:THR:HG22	2.08	0.53
1:A:736:PHE:C	1:A:738:GLN:H	2.16	0.53
1:A:136:ALA:HA	1:A:250:VAL:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:G:H2'	2:B:22:C:H6	1.73	0.53
3:C:13:DT:H2'	3:C:14:DG:H8	1.74	0.53
3:C:5:DC:H2'	3:C:6:DA:C8	2.44	0.52
1:A:1071:ARG:HH11	1:A:1072:PRO:HD2	1.74	0.52
1:A:383:THR:HG22	1:A:424:GLU:OE2	2.10	0.52
2:B:73:C:N4	2:B:92:U:OP2	2.34	0.51
1:A:717:GLU:HB3	1:A:768:LEU:HD11	1.92	0.51
2:B:77:A:H2'	2:B:78:C:C6	2.45	0.51
2:B:55:C:O2'	2:B:56:C:H5'	2.11	0.51
1:A:941:ARG:HB3	1:A:950:PHE:CD1	2.45	0.51
1:A:824:ALA:HB1	1:A:1108:ARG:NH1	2.26	0.51
1:A:899:ILE:HD11	1:A:906:LEU:HD13	1.92	0.51
1:A:1014:PHE:CD2	1:A:1019:VAL:HG22	2.45	0.50
1:A:40:LEU:HD23	1:A:507:TRP:CD2	2.46	0.50
1:A:747:ARG:HH21	1:A:1058:ALA:H	1.59	0.50
1:A:1065:ARG:NH1	1:A:1087:PRO:HG3	2.26	0.50
1:A:1107:ARG:HH22	1:A:1125:TRP:NE1	2.10	0.50
1:A:197:LEU:HD22	1:A:216:PHE:HE2	1.76	0.50
1:A:239:PRO:HG2	1:A:242:VAL:HG22	1.93	0.50
2:B:40:C:H5''	2:B:40:C:H6	1.77	0.50
1:A:144:PRO:HG3	2:B:16:G:H21	1.75	0.50
1:A:1014:PHE:CE2	1:A:1019:VAL:HG22	2.47	0.50
1:A:142:ARG:HG2	1:A:143:ASN:N	2.28	0.49
1:A:987:ALA:HB1	1:A:991:LEU:HD23	1.94	0.49
1:A:872:LEU:O	1:A:875:THR:HG22	2.13	0.49
1:A:941:ARG:HH22	1:A:1130:ALA:H	1.61	0.49
1:A:1090:TRP:CE2	1:A:1092:ALA:HB2	2.48	0.49
1:A:294:LEU:O	1:A:295:ARG:NH1	2.44	0.48
2:B:78:C:H2'	2:B:79:C:H5'	1.95	0.48
2:B:59:C:H4'	2:B:59:C:OP1	2.12	0.48
1:A:759:THR:HB	1:A:807:CYS:SG	2.53	0.48
1:A:831:LEU:HD12	2:B:73:C:H4'	1.96	0.48
1:A:147:THR:H	1:A:150:ASP:HB2	1.77	0.48
1:A:250:VAL:HG13	1:A:251:PHE:CD2	2.48	0.48
2:B:87:G:H2'	2:B:88:G:C8	2.48	0.48
1:A:387:TRP:CD1	1:A:419:HIS:HE2	2.32	0.48
1:A:97:PRO:HG2	1:A:101:VAL:HG13	1.96	0.48
1:A:838:HIS:ND1	1:A:839:GLU:O	2.34	0.48
1:A:729:LEU:HD12	1:A:815:ILE:HD13	1.95	0.48
1:A:804:LYS:HB2	1:A:804:LYS:NZ	2.29	0.48
1:A:1096:LYS:HD2	3:C:-8:DC:H5''	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:CD2	1:A:247:ILE:HG22	2.45	0.47
3:C:9:DA:H2'	3:C:10:DT:C6	2.49	0.47
1:A:900:VAL:HA	1:A:905:VAL:HG12	1.95	0.47
1:A:282:PHE:HA	1:A:445:LEU:HD13	1.96	0.47
1:A:416:LEU:O	1:A:420:LEU:HD21	2.15	0.47
1:A:925:ARG:NH1	2:B:49:A:O3'	2.48	0.47
1:A:178:PRO:HD2	1:A:183:GLN:HE22	1.80	0.47
1:A:951:ALA:HB3	1:A:991:LEU:HD13	1.96	0.47
1:A:145:TRP:NE1	3:C:7:DG:O4'	2.47	0.47
1:A:330:ILE:HD13	1:A:334:ILE:HD12	1.96	0.47
1:A:1012:LEU:HD13	1:A:1103:LEU:HD21	1.96	0.46
1:A:103:PRO:HG2	2:B:28:A:C8	2.50	0.46
1:A:1106:ILE:HG23	1:A:1114:PRO:HB3	1.97	0.46
1:A:338:PRO:HG2	1:A:342:ASP:OD2	2.15	0.46
1:A:457:VAL:CG2	1:A:461:ASN:HB2	2.45	0.46
1:A:233:ALA:HA	1:A:238:LEU:HD12	1.97	0.46
1:A:820:ARG:HB2	1:A:820:ARG:NH1	2.31	0.46
1:A:480:LEU:HD23	1:A:694:ARG:HB3	1.98	0.46
1:A:493:LEU:HG	1:A:497:ARG:NH1	2.30	0.46
1:A:718:ALA:N	1:A:768:LEU:HD21	2.31	0.46
1:A:265:ARG:HD2	1:A:270:PRO:O	2.16	0.46
1:A:1014:PHE:CE1	1:A:1103:LEU:HD11	2.51	0.46
1:A:178:PRO:N	1:A:179:GLY:HA2	2.30	0.45
2:B:26:G:H3'	2:B:27:G:C8	2.51	0.45
1:A:855:LYS:HB3	1:A:855:LYS:HE3	1.65	0.45
1:A:1028:MET:HA	1:A:1031:LYS:HE3	1.99	0.45
1:A:142:ARG:HG2	1:A:143:ASN:H	1.81	0.45
1:A:811:GLY:O	1:A:815:ILE:HG12	2.16	0.45
1:A:879:GLY:HA2	1:A:996:GLU:OE2	2.17	0.45
1:A:506:ARG:HA	1:A:506:ARG:HD2	1.78	0.45
1:A:471:ASP:HA	1:A:472:ASN:HA	1.60	0.45
3:C:10:DT:H2'	3:C:11:DC:O2	2.17	0.45
1:A:1012:LEU:HB3	1:A:1014:PHE:HE1	1.81	0.45
1:A:860:ARG:HH21	1:A:918:ASP:CG	2.26	0.44
1:A:1086:PHE:O	1:A:1087:PRO:C	2.59	0.44
1:A:1107:ARG:HH22	1:A:1125:TRP:CD1	2.36	0.44
1:A:746:ASP:OD2	1:A:748:ARG:NH2	2.46	0.44
2:B:76:C:C2'	2:B:77:A:H5'	2.46	0.44
3:C:-3:DT:H2''	3:C:-2:DA:N7	2.33	0.44
1:A:103:PRO:HB3	2:B:43:C:O2	2.18	0.44
1:A:894:ASP:HB3	1:A:897:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:LEU:HG	1:A:497:ARG:HH11	1.82	0.44
1:A:759:THR:HG21	1:A:810:LEU:HD11	2.00	0.44
1:A:323:ARG:HB2	1:A:363:PHE:CE1	2.52	0.44
1:A:1107:ARG:HH22	1:A:1125:TRP:HE1	1.64	0.44
1:A:441:SER:O	1:A:445:LEU:HG	2.18	0.44
1:A:711:ARG:HA	1:A:712:GLY:HA2	1.59	0.43
1:A:845:PHE:HZ	1:A:923:ARG:HG3	1.82	0.43
2:B:88:G:C2'	2:B:89:G:H5'	2.48	0.43
1:A:1071:ARG:HA	1:A:1071:ARG:HD2	1.91	0.43
2:B:57:U:N3	2:B:59:C:O2	2.51	0.43
1:A:903:ASP:O	1:A:904:ARG:HG3	2.19	0.43
1:A:1026:LEU:HD22	1:A:1090:TRP:NE1	2.33	0.43
2:B:67:C:H2'	2:B:68:G:H5'	1.99	0.43
1:A:716:ALA:HB3	1:A:772:ARG:NH1	2.33	0.43
1:A:268:LEU:HD23	1:A:467:PHE:CD2	2.53	0.43
1:A:1047:LYS:HE2	1:A:1047:LYS:HB3	1.62	0.43
1:A:40:LEU:HD12	1:A:40:LEU:H	1.84	0.43
1:A:942:TRP:HB3	1:A:1000:ALA:HA	1.99	0.43
2:B:81:C:O2'	2:B:82:C:OP1	2.34	0.43
1:A:165:ARG:O	1:A:169:GLU:HG3	2.19	0.43
2:B:81:C:H6	2:B:81:C:C5'	2.31	0.43
1:A:1048:ARG:HG2	1:A:1093:THR:HA	2.00	0.43
1:A:279:CYS:SG	1:A:442:ARG:HG3	2.59	0.43
1:A:423:ALA:HA	1:A:426:GLU:OE1	2.18	0.43
1:A:752:VAL:O	1:A:755:VAL:HG22	2.19	0.43
1:A:84:LEU:O	1:A:88:LEU:HG	2.18	0.42
1:A:301:GLY:HA3	1:A:302:SER:HA	1.81	0.42
1:A:161:TRP:CE2	1:A:181:VAL:HG12	2.54	0.42
1:A:1077:GLU:O	1:A:1081:ILE:HG12	2.19	0.42
2:B:27:G:N2	2:B:42:A:N6	2.63	0.42
2:B:78:C:C2'	2:B:79:C:H5'	2.50	0.42
1:A:820:ARG:HB2	1:A:820:ARG:HH11	1.84	0.42
1:A:1059:GLU:O	1:A:1063:VAL:HG23	2.20	0.42
1:A:1068:ARG:HH11	1:A:1068:ARG:HD2	1.68	0.42
3:C:12:DT:H2'	3:C:13:DT:C6	2.54	0.42
1:A:326:THR:O	1:A:330:ILE:HG12	2.19	0.42
1:A:913:LYS:HB2	1:A:913:LYS:HZ3	1.83	0.42
1:A:1115:ARG:HG2	2:B:94:C:C4	2.54	0.42
3:C:18:DT:C2	3:C:19:DC:C5	3.08	0.42
1:A:40:LEU:HD23	1:A:507:TRP:CE2	2.55	0.42
1:A:770:ASP:HB3	1:A:774:ARG:NE	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:ASP:OD2	1:A:1047:LYS:HG3	2.20	0.42
1:A:221:ARG:HB3	1:A:223:GLU:HG2	2.01	0.42
1:A:457:VAL:HG22	1:A:461:ASN:HB2	2.00	0.42
1:A:872:LEU:HA	1:A:875:THR:HG22	2.01	0.42
3:C:17:DA:H2'	3:C:18:DT:C6	2.55	0.42
3:C:-3:DT:H2''	3:C:-2:DA:C8	2.55	0.41
1:A:96:LEU:HD23	1:A:130:TYR:CD1	2.55	0.41
1:A:418:VAL:O	1:A:420:LEU:HD12	2.20	0.41
2:B:45:U:H2'	2:B:46:A:C8	2.55	0.41
3:C:9:DA:H2'	3:C:10:DT:H6	1.85	0.41
1:A:115:GLU:HG3	1:A:183:GLN:NE2	2.35	0.41
1:A:699:GLY:HA3	1:A:704:VAL:HG22	2.03	0.41
1:A:178:PRO:HD2	1:A:183:GLN:NE2	2.36	0.41
1:A:246:VAL:O	1:A:250:VAL:HG12	2.20	0.41
1:A:473:TRP:HZ3	1:A:476:PRO:HD3	1.85	0.41
1:A:1001:LYS:HE3	1:A:1001:LYS:HB3	1.80	0.41
1:A:824:ALA:HB1	1:A:1108:ARG:HH12	1.86	0.41
1:A:128:LEU:O	1:A:132:VAL:HG22	2.20	0.41
1:A:285:TYR:HA	1:A:449:THR:HG22	2.02	0.41
1:A:287:ILE:HG23	1:A:317:LEU:HD12	2.03	0.41
1:A:374:ILE:O	1:A:378:ARG:HB2	2.20	0.41
1:A:409:ALA:HA	1:A:410:GLY:HA3	1.71	0.41
3:C:-9:DG:H5'	3:C:-9:DG:C8	2.55	0.41
1:A:117:TYR:HA	1:A:236:GLN:OE1	2.21	0.41
3:C:-8:DC:C2'	3:C:-7:DC:H5''	2.44	0.41
1:A:91:LEU:HD12	1:A:91:LEU:HA	1.80	0.40
1:A:136:ALA:CA	1:A:250:VAL:HG23	2.51	0.40
1:A:722:LEU:HD23	1:A:722:LEU:O	2.21	0.40
1:A:941:ARG:HH12	1:A:1128:TRP:C	2.29	0.40
1:A:447:GLY:O	1:A:450:ARG:HG2	2.22	0.40
1:A:1021:THR:HB	1:A:1096:LYS:HE2	2.02	0.40
1:A:1086:PHE:N	1:A:1087:PRO:HD2	2.36	0.40
1:A:948:PRO:HD2	1:A:1128:TRP:CH2	2.56	0.40
3:C:-10:DC:H2''	3:C:-9:DG:C8	2.57	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)
1:A:1117:ARG:NH1	2:B:1:GTP:O5'[3_444]	2.16	0.04

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	932/977 (95%)	870 (93%)	62 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	774/801 (97%)	751 (97%)	23 (3%)	36	68

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	33	GLU
1	A	78	ARG
1	A	108	LEU
1	A	111	LYS
1	A	310	ARG
1	A	341	SER
1	A	354	SER
1	A	393	ARG
1	A	403	LEU
1	A	426	GLU
1	A	482	GLU
1	A	706	GLN

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Mol	Chain	Res	Type
1	A	707	VAL
1	A	816	SER
1	A	855	LYS
1	A	885	SER
1	A	887	SER
1	A	902	SER
1	A	956	SER
1	A	976	GLU
1	A	1001	LYS
1	A	1012	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	GLN
1	A	190	GLN
1	A	198	ASN
1	A	339	ASN
1	A	749	HIS
1	A	1120	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	88/94 (93%)	32 (36%)	2 (2%)

All (32) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	18	U
2	B	19	A
2	B	27	G
2	B	28	A
2	B	35	A
2	B	36	A
2	B	37	A
2	B	38	G
2	B	39	G
2	B	40	C
2	B	49	A

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Mol	Chain	Res	Type
2	B	51	G
2	B	53	C
2	B	54	C
2	B	57	U
2	B	58	U
2	B	59	C
2	B	61	U
2	B	62	G
2	B	63	G
2	B	65	G
2	B	66	U
2	B	69	C
2	B	72	U
2	B	73	C
2	B	77	A
2	B	79	C
2	B	80	C
2	B	81	C
2	B	82	C
2	B	93	U
2	B	94	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	36	A
2	B	81	C

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](#)

There are no ligands in this entry.

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, 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	A	942/977 (96%)	0.75	51 (5%) 31 24	57, 94, 138, 192	0
2	B	90/94 (95%)	0.55	5 (5%) 30 23	66, 97, 241, 272	0
3	C	30/30 (100%)	0.16	0 100 100	71, 81, 100, 110	0
4	D	10/10 (100%)	-0.06	0 100 100	64, 77, 97, 111	0
All	All	1072/1111 (96%)	0.71	56 (5%) 33 26	57, 93, 150, 272	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	416	LEU	4.5
1	A	261	GLU	4.1
1	A	210	LEU	3.6
1	A	76	PHE	3.6
1	A	468	GLY	3.5
1	A	518	GLY	3.4
1	A	301	GLY	3.3
1	A	418	VAL	3.2
1	A	7	GLY	3.2
1	A	421	PRO	3.0
1	A	1087	PRO	2.9
1	A	263	ILE	2.9
1	A	9	VAL	2.7
1	A	778	ALA	2.7
2	B	34	A	2.7
1	A	203	SER	2.7
1	A	473	TRP	2.6
1	A	264	GLY	2.6
1	A	81	LEU	2.6
1	A	72	ARG	2.6
1	A	194	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	459	VAL	2.5
2	B	82	C	2.5
1	A	426	GLU	2.5
1	A	213	ALA	2.5
1	A	482	GLU	2.4
1	A	408	ILE	2.4
1	A	106	ALA	2.4
1	A	490	ASP	2.3
1	A	187	TYR	2.3
1	A	307	LEU	2.3
1	A	211	SER	2.3
1	A	302	SER	2.3
1	A	481	HIS	2.3
1	A	423	ALA	2.3
1	A	469	VAL	2.2
2	B	58	U	2.2
1	A	820	ARG	2.2
1	A	486	HIS	2.2
1	A	299	GLY	2.2
1	A	1023	ALA	2.2
1	A	968	ASP	2.2
1	A	484	THR	2.2
1	A	262	ARG	2.1
1	A	1117	ARG	2.1
1	A	134	HIS	2.1
1	A	1027	SER	2.1
1	A	99	LYS	2.1
1	A	1102	GLY	2.1
1	A	257	SER	2.1
1	A	1072	PRO	2.0
2	B	88	G	2.0
1	A	470	ASP	2.0
1	A	1066	THR	2.0
1	A	32	GLU	2.0
2	B	65	G	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.