Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2024 – 08:37 AM EST

PDB ID	:	6WBR
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:

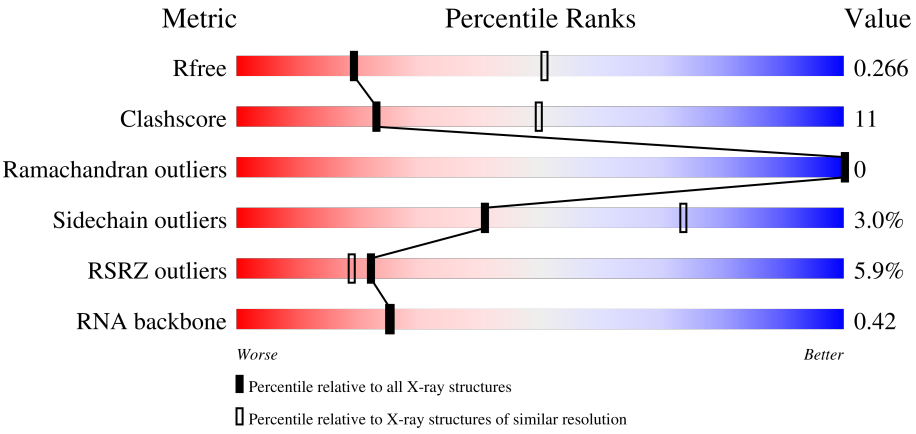
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)
RNA backbone	3102	1001 (3.18-2.66)

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 <=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	13% 37% 33% 21% 5%
3	C	30	33% 53% 13%
4	D	10	100%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	942	7400	4653	1377	1357	13	0	0	0

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
			Total	C	N	O	P			
2	B	91	1952	866	348	645	93	9	0	0

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

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

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

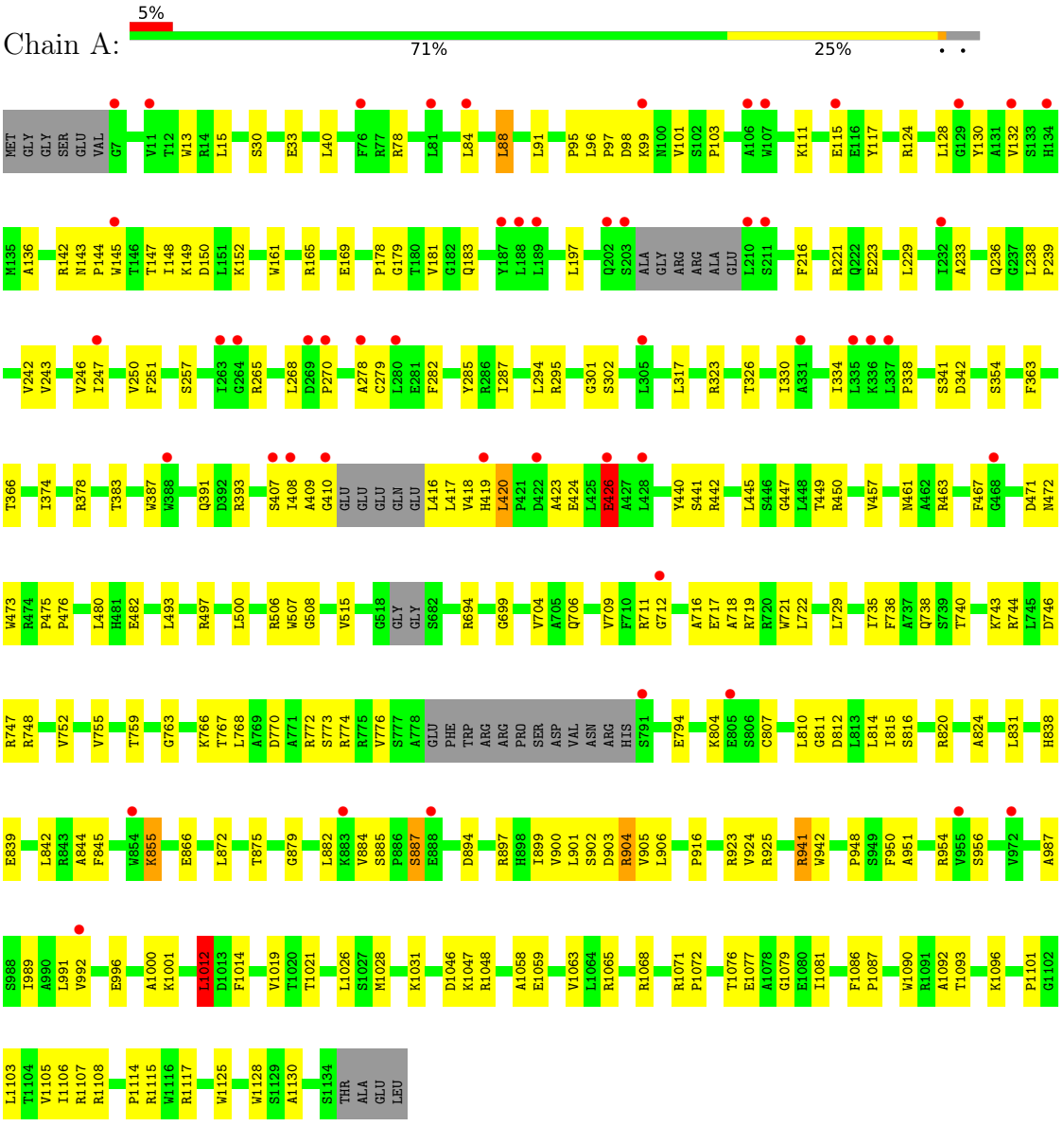
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	10	Total	C	N	O	P	0	0	0
			202	97	38	58	9			

3 Residue-property plots (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.

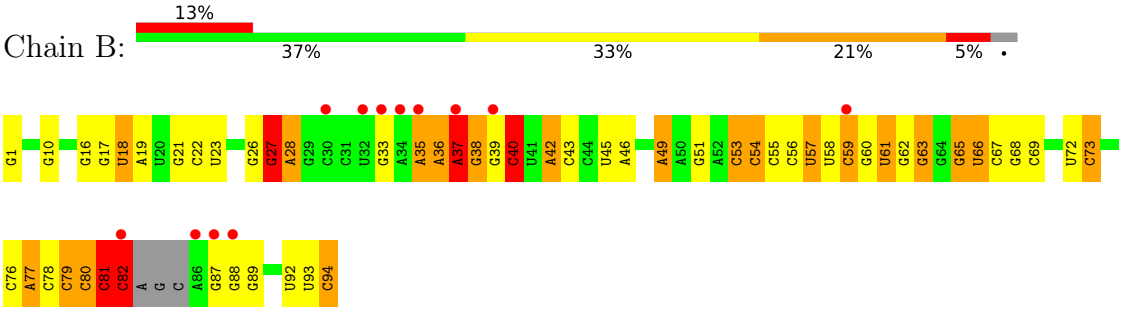
• Molecule 1: CRISPR-associated endonuclease, Csn1 family,CRISPR-associated endonuclease, Csn1 family

Chain A:



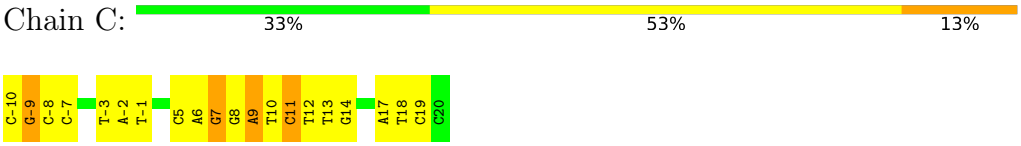
• Molecule 2: RNA (94-MER)

Chain B:



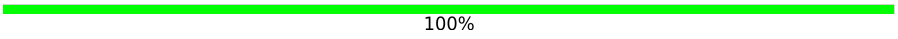
• Molecule 3: DNA (30-MER)

Chain C:



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

Chain D:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

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 98.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.2 (74.65-2.91) 92.0 (98.99-2.90)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.71 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.224 , 0.266 0.224 , 0.266	Depositor DCC
R_{free} test set	1901 reflections (4.87%)	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 , 57.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.36	0/7567	0.63	3/10285 (0.0%)
2	B	0.52	0/2144	1.26	25/3338 (0.7%)
3	C	0.92	1/678 (0.1%)	1.10	3/1043 (0.3%)
4	D	0.86	0/226	0.98	0/347
All	All	0.47	1/10615 (0.0%)	0.85	31/15013 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	9	DA	C3'-O3'	-5.16	1.37	1.44

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	7	DG	O4'-C1'-N9	8.80	114.16	108.00
2	B	53	C	C2-N1-C1'	7.73	127.30	118.80
2	B	53	C	C6-N1-C1'	-7.23	112.12	120.80
2	B	40	C	C6-N1-C2	-7.06	117.48	120.30
3	C	11	DC	O4'-C1'-N1	6.62	112.63	108.00
2	B	65	G	N9-C4-C5	-6.51	102.80	105.40
2	B	63	G	N3-C4-N9	6.35	129.81	126.00
1	A	420	LEU	CA-CB-CG	6.30	129.79	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	65	G	C4-C5-N7	6.23	113.29	110.80
2	B	81	C	C5-C6-N1	6.15	124.07	121.00
2	B	40	C	C5-C6-N1	6.01	124.01	121.00
3	C	-9	DG	O4'-C4'-C3'	-5.95	102.12	104.50
2	B	66	U	C2-N1-C1'	5.90	124.78	117.70
1	A	426	GLU	CA-CB-CG	5.89	126.36	113.40
2	B	63	G	C6-C5-N7	-5.76	126.94	130.40
2	B	66	U	C5-C4-O4	-5.73	122.46	125.90
2	B	82	C	C2-N1-C1'	5.71	125.08	118.80
2	B	63	G	C4-N9-C1'	5.71	133.92	126.50
2	B	27	G	N3-C2-N2	-5.65	115.94	119.90
2	B	27	G	N3-C4-N9	-5.63	122.62	126.00
2	B	42	A	N9-C4-C5	-5.58	103.57	105.80
2	B	42	A	N1-C6-N6	5.45	121.87	118.60
2	B	63	G	C8-N9-C1'	-5.43	119.94	127.00
2	B	37	A	O4'-C1'-N9	5.36	112.49	108.20
2	B	81	C	C6-N1-C2	-5.28	118.19	120.30
2	B	66	U	C5-C6-N1	5.26	125.33	122.70
2	B	80	C	C2-N1-C1'	5.24	124.57	118.80
2	B	54	C	C5-C6-N1	5.16	123.58	121.00
1	A	1012	LEU	CA-CB-CG	5.11	127.05	115.30
2	B	82	C	C5-C6-N1	5.07	123.54	121.00
2	B	36	A	P-O3'-C3'	5.00	125.70	119.70

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7400	0	7379	165	1
2	B	1952	0	984	40	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	606	0	339	21	0
4	D	202	0	114	0	0
All	All	10160	0	8816	216	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 11.

All (216) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:736:PHE:HD2	1:A:740:THR:HG1	1.56	0.53
1:A:763:GLY:O	1:A:767:THR:HG22	2.08	0.53
1:A:136:ALA:HA	1:A:250:VAL:HG23	1.91	0.53
1:A:98:ASP:HB2	1:A:99:LYS:HZ2	1.73	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:887:SER:O	1:A:887:SER:OG	2.23	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:736:PHE:C	1:A:738:GLN:H	2.16	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:37:A:HO2'	2:B:38:G:H8	1.67	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: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 (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
1	A	932/977 (95%)	870 (93%)	62 (7%)	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
1	A	774/801 (97%)	751 (97%)	23 (3%)	41 73

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

Mol	Chain	Res	Type
1	A	78	ARG
1	A	88	LEU
1	A	111	LYS
1	A	341	SER
1	A	354	SER
1	A	393	ARG
1	A	426	GLU
1	A	482	GLU
1	A	706	GLN
1	A	721	TRP
1	A	744	ARG
1	A	794	GLU
1	A	812	ASP
1	A	816	SER
1	A	855	LYS
1	A	885	SER
1	A	887	SER
1	A	902	SER
1	A	904	ARG
1	A	941	ARG
1	A	954	ARG
1	A	956	SER
1	A	1012	LEU

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

5.3.3 RNA (i)

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
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 monosaccharides 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, 95^{th} 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%)	0.73	51 (5%) 25 22	57, 94, 138, 192	0
2	B	90/94 (95%)	1.00	12 (13%) 3 2	66, 97, 241, 272	0
3	C	30/30 (100%)	0.08	0 100 100	71, 81, 100, 110	0
4	D	10/10 (100%)	-0.04	0 100 100	64, 77, 97, 111	0
All	All	1072/1111 (96%)	0.73	63 (5%) 22 19	57, 93, 150, 272	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	SER	7.0
2	B	34	A	7.0
1	A	203	SER	6.9
1	A	408	ILE	4.8
1	A	211	SER	4.3
1	A	791	SER	4.2
2	B	87	G	4.0
2	B	32	U	3.5
1	A	76	PHE	3.5
1	A	81	LEU	3.5
1	A	419	HIS	3.4
2	B	86	A	3.3
2	B	35	A	3.2
1	A	189	LEU	3.0
1	A	335	LEU	2.9
1	A	7	GLY	2.9
1	A	210	LEU	2.8
1	A	336	LYS	2.8
1	A	305	LEU	2.8
1	A	468	GLY	2.8
1	A	84	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	37	A	2.7
1	A	188	LEU	2.7
1	A	410	GLY	2.7
1	A	263	ILE	2.7
1	A	280	LEU	2.6
2	B	82	C	2.6
1	A	426	GLU	2.6
2	B	88	G	2.5
1	A	428	LEU	2.5
1	A	115	GLU	2.5
1	A	99	LYS	2.5
2	B	33	G	2.5
2	B	59	C	2.4
1	A	972	VAL	2.4
1	A	187	TYR	2.4
1	A	888	GLU	2.3
1	A	232	ILE	2.3
1	A	337	LEU	2.3
1	A	955	VAL	2.3
1	A	145	TRP	2.3
1	A	331	ALA	2.3
1	A	805	GLU	2.3
1	A	134	HIS	2.2
2	B	30	C	2.2
1	A	854	TRP	2.2
1	A	247	ILE	2.1
1	A	264	GLY	2.1
2	B	39	G	2.1
1	A	712	GLY	2.1
1	A	992	VAL	2.1
1	A	278	ALA	2.1
1	A	270	PRO	2.1
1	A	202	GLN	2.1
1	A	11	VAL	2.1
1	A	269	ASP	2.0
1	A	106	ALA	2.0
1	A	129	GLY	2.0
1	A	132	VAL	2.0
1	A	422	ASP	2.0
1	A	107	TRP	2.0
1	A	388	TRP	2.0
1	A	883	LYS	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 monosaccharides 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.