



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:32 PM EDT

PDB ID : 8HNW / pdb_00008hnw
Title : Crystal structure of HpaCas9-sgRNA surveillance complex bound to double-stranded DNA
Authors : Sun, W.; Cheng, Z.; Wang, Y.
Deposited on : 2022-12-08
Resolution : 3.41 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

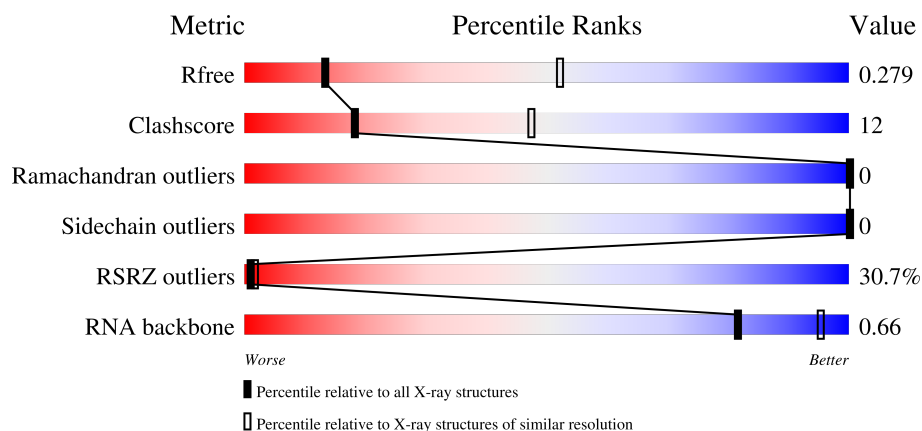
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)
RNA backbone	3983	1162 (3.84-3.00)

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	1055	24% 56% 20% 23%
2	B	128	26% 36% 45% 16%
3	C	35	14% 43% 57%
4	D	11	27% 100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9266 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 Cas9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	809	Total	C	N	O	S	0	1	0
			6071	3867	1084	1100	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP F0ET08
A	581	ALA	HIS	engineered mutation	UNP F0ET08

- Molecule 2 is a RNA chain called sgRNA.

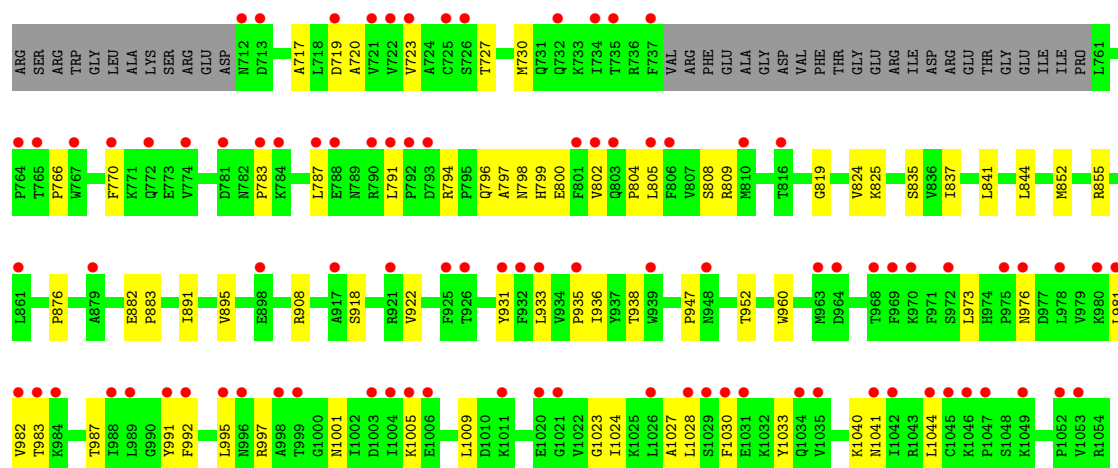
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	107	Total	C	N	O	P	0	0	0
			2251	1010	380	754	107			

- Molecule 3 is a DNA chain called Target strand.

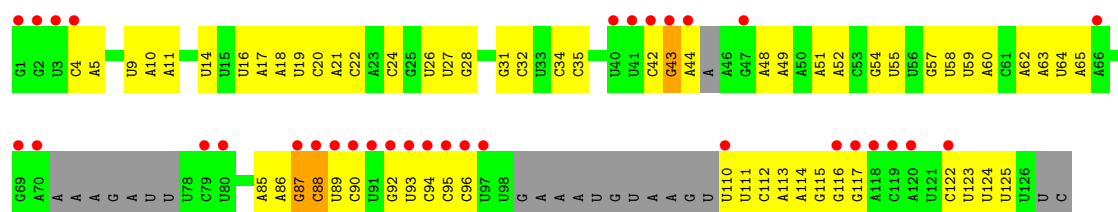
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	35	Total	C	N	O	P	0	0	0
			721	347	133	207	34			

- Molecule 4 is a DNA chain called Non-target strand.

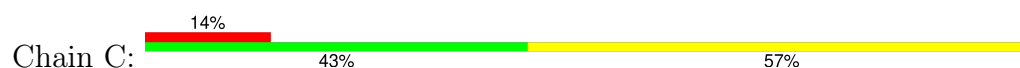
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total	C	N	O	P	0	0	0
			223	110	37	66	10			



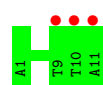
• Molecule 2: sgRNA



• Molecule 3: Target strand



• Molecule 4: Non-target strand



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	158.87Å 185.76Å 160.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.62 – 3.41 44.62 – 3.41	Depositor EDS
% Data completeness (in resolution range)	73.6 (44.62-3.41) 74.1 (44.62-3.41)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.78 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.258 , 0.281 0.256 , 0.279	Depositor DCC
R_{free} test set	1185 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 97.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	9266	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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](#)

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	0.13	0/6172	0.35	0/8365
2	B	0.11	0/2508	0.26	0/3891
3	C	0.20	0/810	0.40	0/1250
4	D	0.19	0/249	0.44	0/383
All	All	0.13	0/9739	0.34	0/13889

There are no bond length outliers.

There are no bond angle outliers.

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	A	6071	0	5880	147	0
2	B	2251	0	1146	55	0
3	C	721	0	399	20	0
4	D	223	0	129	0	0
All	All	9266	0	7554	203	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 (203) 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)
1:A:77:LYS:HG3	1:A:81:ARG:HH21	1.48	0.79
1:A:368:ASN:HB3	1:A:371:LEU:HB2	1.64	0.77
2:B:113:A:H2'	2:B:114:A:H8	1.52	0.73
1:A:104:ARG:NH2	1:A:201:GLU:OE1	2.24	0.71
1:A:60:ARG:NH1	2:B:18:A:OP2	2.24	0.71
1:A:242:LEU:HG	1:A:381:LEU:HD21	1.73	0.70
1:A:306:TYR:HD2	1:A:336:THR:HG23	1.56	0.70
2:B:112:C:H2'	2:B:113:A:H8	1.57	0.69
1:A:166:SER:HB2	1:A:201:GLU:HG3	1.74	0.69
2:B:113:A:H2'	2:B:114:A:C8	2.29	0.68
1:A:78:LYS:HD3	1:A:228:LEU:HD11	1.77	0.66
1:A:145:LEU:HD22	1:A:149:LEU:HB3	1.78	0.66
1:A:92:THR:HG22	1:A:93:ASP:H	1.61	0.64
1:A:799:HIS:HB3	1:A:802:VAL:HG23	1.79	0.63
2:B:85:A:H2'	2:B:86:A:C8	2.34	0.62
1:A:291:ARG:O	1:A:295:MET:N	2.32	0.62
2:B:112:C:H2'	2:B:113:A:C8	2.34	0.62
1:A:100:VAL:HG11	1:A:123:HIS:CG	2.34	0.62
1:A:104:ARG:HG2	1:A:120:VAL:HG13	1.82	0.62
1:A:825:LYS:HG2	1:A:837:ILE:HB	1.82	0.61
1:A:882:GLU:HG3	1:A:883:PRO:HD2	1.82	0.61
3:C:23:DT:H2'	3:C:24:DG:H8	1.66	0.61
1:A:495:HIS:HB3	1:A:723:VAL:HG12	1.83	0.61
1:A:253:GLU:HB3	1:A:417:SER:HB3	1.83	0.60
1:A:766:PRO:HD2	1:A:770:PHE:CZ	2.36	0.60
1:A:241:ILE:HD12	1:A:241:ILE:H	1.65	0.60
1:A:9:ILE:HA	1:A:492:ALA:HB3	1.84	0.59
1:A:265:ARG:HB3	1:A:425:LEU:HD11	1.84	0.59
1:A:981:LEU:HD13	1:A:1030:PHE:HD1	1.66	0.59
1:A:75:ARG:HG3	1:A:228:LEU:HD12	1.85	0.59
1:A:71:ARG:NH1	2:B:21:A:OP2	2.37	0.58
1:A:783:PRO:HB3	1:A:804:PRO:HD3	1.84	0.58
1:A:258:LYS:HB3	1:A:412:LYS:HB2	1.84	0.57
1:A:908:ARG:NH2	2:B:64:U:O2'	2.37	0.57
2:B:4:C:H2'	2:B:5:A:C8	2.40	0.57
1:A:19:VAL:HG23	1:A:43:PHE:HE1	1.69	0.56
1:A:717:ALA:O	1:A:720:ALA:HB3	2.04	0.56
1:A:824:VAL:O	2:B:26:U:O2'	2.22	0.56
1:A:148:LEU:HB3	3:C:16:DG:H5''	1.87	0.56
1:A:164:TYR:HB3	1:A:170:LEU:HB2	1.86	0.56
1:A:171:ALA:HB1	1:A:182:ILE:HG23	1.87	0.56
1:A:299:TYR:CE2	1:A:343:MET:HE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:ASN:N	1:A:992:PHE:O	2.40	0.55
1:A:1033:TYR:CZ	1:A:1044:LEU:HD13	2.41	0.55
1:A:184:ASN:HB2	2:B:24:C:O5'	2.06	0.55
1:A:362:TRP:O	1:A:366:LYS:N	2.39	0.55
2:B:92:G:H2'	2:B:93:U:H6	1.72	0.55
2:B:48:A:H2'	2:B:49:A:C8	2.42	0.55
1:A:277:ILE:HB	1:A:284:ARG:HG3	1.88	0.55
1:A:799:HIS:CG	1:A:800:GLU:N	2.75	0.55
2:B:114:A:H2'	2:B:115:G:H8	1.72	0.55
1:A:71:ARG:NH2	2:B:20:C:OP1	2.36	0.54
1:A:973:LEU:HD11	1:A:1030:PHE:HE2	1.71	0.54
1:A:269:ILE:HD12	1:A:428:MET:HB2	1.90	0.54
2:B:92:G:H2'	2:B:93:U:C6	2.42	0.54
1:A:347:HIS:HA	1:A:350:ARG:HG2	1.90	0.54
3:C:23:DT:H2'	3:C:24:DG:C8	2.42	0.54
1:A:662:ASP:O	1:A:666:VAL:HG23	2.08	0.54
1:A:190:THR:HG23	1:A:191:HIS:HD2	1.73	0.53
1:A:349:ILE:HD13	1:A:375:ILE:HD11	1.90	0.53
1:A:117:TRP:O	1:A:121:LEU:HG	2.08	0.53
2:B:4:C:H2'	2:B:5:A:H8	1.72	0.53
1:A:1040:LYS:HG3	1:A:1041:ASN:H	1.74	0.52
3:C:7:DC:H4'	3:C:8:DA:OP1	2.10	0.52
1:A:220:LYS:H	1:A:220:LYS:HD2	1.74	0.52
1:A:206:PHE:O	1:A:210:GLN:HG3	2.09	0.52
1:A:234:PRO:HG2	1:A:237:SER:HB3	1.92	0.51
2:B:16:U:H2'	2:B:17:A:H8	1.75	0.51
2:B:51:A:H2'	2:B:52:A:H8	1.75	0.51
2:B:85:A:H2'	2:B:86:A:H8	1.75	0.51
1:A:370:THR:O	1:A:374:GLU:HG2	2.11	0.51
1:A:62:ALA:O	1:A:66:ARG:HG3	2.10	0.50
1:A:270:THR:O	1:A:274:ASN:ND2	2.44	0.50
1:A:362:TRP:O	1:A:366:LYS:HG3	2.10	0.50
1:A:852:MET:HE3	1:A:895:VAL:HB	1.93	0.50
2:B:16:U:H2'	2:B:17:A:C8	2.46	0.50
1:A:67:ARG:HH12	2:B:19:U:H5''	1.75	0.50
1:A:825:LYS:HD2	1:A:835:SER:OG	2.11	0.50
1:A:83:LEU:HD22	1:A:88:ILE:HD12	1.94	0.50
2:B:51:A:H2'	2:B:52:A:C8	2.47	0.50
1:A:371:LEU:O	1:A:375:ILE:HG23	2.11	0.49
1:A:39:GLY:HA2	1:A:805:LEU:CD1	2.41	0.49
1:A:124:LEU:O	1:A:229:LEU:HD13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:HD22	1:A:204:LEU:HD22	1.93	0.49
1:A:294:LEU:HD21	1:A:309:VAL:HG13	1.93	0.49
1:A:16:ILE:HA	1:A:473:THR:HG21	1.93	0.49
1:A:298:PRO:HD3	1:A:304:LEU:HD22	1.93	0.49
1:A:21:TRP:CE2	1:A:39:GLY:HA3	2.48	0.49
1:A:199:LEU:O	1:A:203:GLU:HG3	2.13	0.49
1:A:306:TYR:CD2	1:A:336:THR:HG23	2.42	0.49
1:A:96:LEU:HB3	1:A:119:ALA:HB2	1.95	0.49
2:B:110:U:H2'	2:B:111:U:C6	2.48	0.48
1:A:39:GLY:HA2	1:A:805:LEU:HD11	1.96	0.48
1:A:935:PRO:HB3	1:A:995:LEU:HD23	1.95	0.48
2:B:10:A:H2'	2:B:11:A:C8	2.48	0.48
2:B:122:C:H2'	2:B:123:U:C6	2.49	0.48
1:A:982:VAL:HG12	1:A:987:THR:HB	1.96	0.48
2:B:124:U:H2'	2:B:125:U:C6	2.49	0.48
2:B:54:G:H2'	2:B:55:U:O4'	2.14	0.48
2:B:123:U:H2'	2:B:124:U:C6	2.49	0.47
3:C:9:DT:H2''	3:C:10:DA:H8	1.78	0.47
1:A:1005:LYS:HD2	1:A:1009:LEU:HD21	1.96	0.47
2:B:115:G:H2'	2:B:116:G:C8	2.48	0.47
2:B:42:C:H2'	2:B:43:G:O4'	2.15	0.47
2:B:114:A:H2'	2:B:115:G:C8	2.49	0.47
1:A:470:VAL:HG13	1:A:666:VAL:HG22	1.97	0.47
1:A:719:ASP:O	1:A:723:VAL:HG23	2.14	0.47
2:B:86:A:H2'	2:B:87:G:C8	2.49	0.47
1:A:344:LYS:O	1:A:348:GLN:HG3	2.14	0.47
1:A:14:LEU:HD13	1:A:666:VAL:HG12	1.97	0.47
1:A:852:MET:O	1:A:855[B]:ARG:NH1	2.48	0.47
1:A:891:ILE:HG23	2:B:57:G:H4'	1.97	0.47
3:C:26:DT:H2'	3:C:27:DA:H8	1.80	0.46
1:A:273:ASN:O	1:A:276:ARG:NH2	2.48	0.46
3:C:22:DA:H2'	3:C:23:DT:C6	2.50	0.46
1:A:475:THR:OG1	2:B:87:G:OP1	2.32	0.46
1:A:799:HIS:CG	1:A:800:GLU:H	2.33	0.46
1:A:883:PRO:HB3	1:A:891:ILE:HD11	1.96	0.46
1:A:378:ALA:HB2	1:A:391:TYR:CD1	2.51	0.46
1:A:983:THR:HG22	1:A:1027:ALA:HA	1.97	0.46
3:C:1:DT:H2''	3:C:2:DA:C8	2.50	0.46
1:A:41:ARG:NH1	1:A:808:SER:OG	2.47	0.46
1:A:665:TYR:CZ	3:C:22:DA:H4'	2.51	0.46
1:A:973:LEU:HD11	1:A:1030:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:DT:H1'	3:C:16:DG:H5'	1.97	0.46
1:A:239:GLU:O	1:A:243:LYS:HG3	2.16	0.45
1:A:819:GLY:HA2	1:A:938:THR:HB	1.98	0.45
3:C:25:DT:H2'	3:C:26:DT:C6	2.52	0.45
2:B:59:U:H2'	2:B:60:A:H8	1.81	0.45
1:A:121:LEU:O	1:A:125:ILE:HG12	2.15	0.45
3:C:3:DA:H1'	3:C:4:DA:H5'	1.99	0.45
1:A:960:TRP:HH2	1:A:997:ARG:HG3	1.81	0.45
1:A:427:LEU:HD11	1:A:441:ILE:HD11	1.99	0.45
1:A:16:ILE:HG23	1:A:663:THR:HG22	1.98	0.44
1:A:922:VAL:HG11	1:A:933:LEU:HD23	1.99	0.44
1:A:983:THR:HA	1:A:1028:LEU:HG	1.98	0.44
3:C:19:DT:H2'	3:C:20:DA:C8	2.52	0.44
3:C:9:DT:H2''	3:C:10:DA:C8	2.52	0.44
1:A:306:TYR:CZ	1:A:321:PHE:HD2	2.36	0.44
2:B:59:U:H2'	2:B:60:A:C8	2.53	0.44
2:B:110:U:H2'	2:B:111:U:H6	1.83	0.44
1:A:181:HIS:HB3	2:B:58:U:H5''	1.99	0.44
2:B:111:U:H2'	2:B:112:C:C6	2.53	0.44
1:A:467:ASN:HD22	1:A:468:PRO:HD2	1.82	0.44
2:B:93:U:H2'	2:B:94:C:H6	1.83	0.44
1:A:135:LYS:NZ	1:A:411:ASP:OD2	2.45	0.44
1:A:384:THR:O	1:A:388:ILE:HG13	2.18	0.44
1:A:203:GLU:HA	1:A:222:LEU:HD11	2.00	0.44
2:B:62:A:H2'	2:B:63:A:H8	1.82	0.44
1:A:358:LEU:HD13	1:A:400:VAL:HG22	2.00	0.43
1:A:1023:GLY:N	3:C:5:DA:OP2	2.39	0.43
2:B:31:G:H2'	2:B:32:C:C6	2.53	0.43
2:B:34:C:H2'	2:B:35:C:O4'	2.19	0.43
1:A:353:LEU:HD21	1:A:400:VAL:HG13	1.99	0.43
1:A:305:PHE:HB2	1:A:308:GLN:HG3	2.00	0.43
1:A:441:ILE:O	1:A:441:ILE:HG22	2.18	0.43
1:A:918:SER:OG	1:A:938:THR:OG1	2.36	0.43
1:A:88:ILE:O	1:A:114:ARG:NE	2.52	0.43
1:A:794:ARG:C	1:A:796:GLN:H	2.27	0.43
1:A:1001:ASN:ND2	3:C:5:DA:N7	2.66	0.43
1:A:922:VAL:O	1:A:973:LEU:N	2.52	0.43
1:A:100:VAL:HG11	1:A:123:HIS:CB	2.49	0.43
1:A:105:VAL:HG13	1:A:169:GLU:HG3	2.01	0.42
1:A:117:TRP:NE1	1:A:121:LEU:HD11	2.33	0.42
1:A:262:SER:OG	1:A:373:ASP:OD2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:HG	1:A:491:PRO:HG2	2.02	0.42
1:A:727:THR:HG22	1:A:730:MET:HE2	2.02	0.42
3:C:26:DT:H2'	3:C:27:DA:C8	2.54	0.42
1:A:787:LEU:O	1:A:791:LEU:N	2.53	0.42
1:A:936:ILE:HG12	1:A:947:PRO:HG2	2.01	0.42
2:B:87:G:N2	2:B:123:U:C2	2.87	0.42
2:B:87:G:H2'	2:B:88:C:C6	2.55	0.42
1:A:135:LYS:HG3	3:C:18:DT:OP1	2.20	0.42
1:A:220:LYS:O	1:A:224:ASN:ND2	2.45	0.42
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.89	0.42
2:B:58:U:H2'	2:B:59:U:C6	2.54	0.42
1:A:661:ASN:ND2	2:B:14:U:O2	2.53	0.42
1:A:952:THR:HB	1:A:960:TRP:CD1	2.55	0.42
1:A:350:ARG:O	1:A:354:GLU:N	2.24	0.41
1:A:411:ASP:HB3	3:C:19:DT:OP1	2.20	0.41
1:A:692:ASN:O	1:A:696:THR:HG23	2.20	0.41
1:A:797:ALA:O	1:A:798:ASN:HB3	2.20	0.41
2:B:9:U:H2'	2:B:10:A:C8	2.55	0.41
2:B:95:C:H2'	2:B:96:C:H6	1.85	0.41
1:A:844:LEU:C	1:A:876:PRO:HG3	2.45	0.41
2:B:27:U:H2'	2:B:28:G:H8	1.86	0.41
1:A:766:PRO:HD2	1:A:770:PHE:HZ	1.82	0.41
1:A:809:ARG:HD2	1:A:991:TYR:CD2	2.56	0.41
2:B:95:C:H2'	2:B:96:C:C6	2.56	0.41
1:A:129:GLY:O	2:B:22:C:H4'	2.20	0.41
1:A:430:GLN:NE2	1:A:430:GLN:HA	2.36	0.41
1:A:168:ALA:O	1:A:172:VAL:HG23	2.20	0.41
1:A:411:ASP:C	1:A:412:LYS:HD2	2.46	0.41
1:A:931:TYR:HB2	1:A:1024:ILE:O	2.20	0.41
3:C:24:DG:H2'	3:C:25:DT:C6	2.56	0.41
1:A:67:ARG:HH11	2:B:20:C:P	2.44	0.41
1:A:350:ARG:HG3	1:A:351:LYS:N	2.36	0.41
1:A:295:MET:HE2	1:A:295:MET:HB2	1.93	0.40
1:A:679:HIS:CG	1:A:680:LEU:N	2.90	0.40
1:A:421:LEU:HD23	1:A:421:LEU:HA	1.95	0.40
1:A:841:LEU:HD23	1:A:841:LEU:HA	1.91	0.40
1:A:418:LEU:HD12	1:A:421:LEU:HD12	2.03	0.40
2:B:89:U:H2'	2:B:90:C:H6	1.87	0.40

There are no symmetry-related clashes.

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	788/1055 (75%)	731 (93%)	57 (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	593/918 (65%)	593 (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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	HIS
1	A	211	HIS
1	A	368	ASN
1	A	430	GLN
1	A	467	ASN
1	A	818	GLN
1	A	911	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	103/128 (80%)	5 (4%)	1 (0%)

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	43	G
2	B	44	A
2	B	65	A
2	B	88	C
2	B	117	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	87	G

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	809/1055 (76%)	1.69	254 (31%)  	5, 58, 99, 129	1 (0%)
2	B	107/128 (83%)	1.42	33 (30%)  	7, 56, 159, 190	0
3	C	35/35 (100%)	1.23	5 (14%)  	13, 44, 80, 83	0
4	D	11/11 (100%)	1.18	3 (27%)  	25, 29, 75, 76	0
All	All	962/1229 (78%)	1.64	295 (30%)  	5, 57, 105, 190	1 (0%)

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	TYR	9.0
1	A	22	ALA	8.1
1	A	806	PHE	6.8
1	A	1045	CYS	6.8
1	A	132	SER	6.3
1	A	695	ILE	6.2
1	A	388	ILE	6.0
1	A	375	ILE	5.8
1	A	376	GLY	5.8
1	A	661	ASN	5.7
1	A	790	ARG	5.6
2	B	117	G	5.5
1	A	1034	GLN	5.4
1	A	392	LEU	5.2
1	A	246	GLY	5.0
1	A	130	TYR	5.0
1	A	774	VAL	4.9
1	A	289	ASN	4.8
1	A	791	LEU	4.8
3	C	4	DA	4.7
1	A	801	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	431	GLY	4.6
1	A	991	TYR	4.5
1	A	31	ASN	4.5
1	A	144	GLU	4.5
1	A	792	PRO	4.4
1	A	30	GLU	4.3
1	A	438	CYS	4.3
1	A	85	SER	4.2
1	A	55	LEU	4.1
2	B	80	U	4.1
1	A	371	LEU	4.1
1	A	659	ASN	4.0
1	A	803	GLN	4.0
1	A	491	PRO	4.0
1	A	436	GLU	4.0
1	A	732	GLN	4.0
1	A	1030	PHE	4.0
1	A	306	TYR	4.0
1	A	23	VAL	4.0
1	A	275	LEU	4.0
1	A	999	THR	3.9
1	A	251	GLU	3.9
1	A	721	VAL	3.9
1	A	725	CYS	3.9
2	B	94	C	3.9
1	A	37	ASP	3.8
1	A	998	ALA	3.7
1	A	1035	VAL	3.7
2	B	42	C	3.7
1	A	346	TYR	3.6
1	A	370	THR	3.6
1	A	473	THR	3.6
1	A	24	VAL	3.6
1	A	393	ALA	3.5
1	A	153	ASP	3.5
1	A	415	GLN	3.5
1	A	673	PHE	3.5
1	A	372	LEU	3.5
1	A	296	GLU	3.4
1	A	428	MET	3.4
1	A	805	LEU	3.4
1	A	1047	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	88	C	3.4
1	A	1004	ILE	3.4
1	A	92	THR	3.4
1	A	669	PHE	3.3
1	A	421	LEU	3.3
2	B	95	C	3.3
4	D	11	DA	3.3
1	A	277	ILE	3.3
1	A	719	ASP	3.3
1	A	32	PRO	3.3
1	A	192	THR	3.3
2	B	1	G	3.3
1	A	16	ILE	3.3
1	A	218	SER	3.2
1	A	879	ALA	3.2
1	A	268	TRP	3.2
1	A	342	GLU	3.2
1	A	989	LEU	3.2
1	A	91	SER	3.2
1	A	456	PHE	3.2
1	A	992	PHE	3.2
1	A	98	HIS	3.2
1	A	980	LYS	3.2
1	A	1044	LEU	3.2
1	A	737	PHE	3.2
1	A	1003	ASP	3.2
1	A	481	ILE	3.2
1	A	131	LEU	3.1
2	B	92	G	3.1
1	A	713	ASP	3.1
2	B	119	C	3.1
1	A	161	GLN	3.1
1	A	417	SER	3.1
1	A	460	ILE	3.1
1	A	963	MET	3.1
1	A	250	PHE	3.1
1	A	1006	GLU	3.1
3	C	30	DG	3.0
2	B	93	U	3.0
1	A	982	VAL	3.0
2	B	97	U	3.0
2	B	116	G	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	86	GLU	3.0
1	A	208	ARG	3.0
2	B	79	C	3.0
1	A	696	THR	3.0
1	A	690	ALA	2.9
1	A	236	LEU	2.9
1	A	418	LEU	2.9
1	A	935	PRO	2.9
1	A	254	TYR	2.9
1	A	793	ASP	2.9
1	A	265	ARG	2.9
2	B	70	A	2.9
1	A	783	PRO	2.9
2	B	96	C	2.9
1	A	726	SER	2.9
1	A	767	TRP	2.9
1	A	931	TYR	2.9
1	A	675	ALA	2.9
1	A	1053	VAL	2.9
1	A	110	HIS	2.8
1	A	361	GLU	2.8
1	A	485	VAL	2.8
2	B	90	C	2.8
1	A	419	LYS	2.8
1	A	1005	LYS	2.8
1	A	983	THR	2.8
1	A	129	GLY	2.8
1	A	70	GLN	2.8
1	A	133	GLN	2.8
1	A	292	LEU	2.8
1	A	93	ASP	2.8
1	A	674	ILE	2.8
1	A	15	GLY	2.7
1	A	676	ASP	2.7
1	A	116	GLU	2.7
1	A	266	PHE	2.7
1	A	770	PHE	2.7
1	A	1029	SER	2.7
1	A	926	THR	2.7
1	A	772	GLN	2.7
1	A	364	GLU	2.7
1	A	442	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	976	ASN	2.7
1	A	995	LEU	2.7
1	A	1042	ILE	2.7
1	A	693	GLY	2.7
1	A	138	SER	2.7
1	A	19	VAL	2.7
1	A	352	VAL	2.7
1	A	193	PHE	2.6
1	A	466	ARG	2.6
1	A	1046	LYS	2.6
1	A	475	THR	2.6
1	A	285	ALA	2.6
1	A	396	LEU	2.6
1	A	699	LEU	2.6
1	A	94	GLU	2.6
1	A	295	MET	2.6
1	A	99	GLN	2.6
2	B	40	U	2.6
2	B	43	G	2.6
1	A	996	ASN	2.6
1	A	221	LEU	2.6
1	A	975	PRO	2.6
1	A	898	GLU	2.6
1	A	764	PRO	2.5
1	A	282	LEU	2.5
1	A	978	LEU	2.5
1	A	226	THR	2.5
1	A	382	TYR	2.5
1	A	337	LYS	2.5
1	A	981	LEU	2.5
2	B	3	U	2.5
1	A	781	ASP	2.5
1	A	391	TYR	2.5
1	A	921	ARG	2.5
1	A	109	ASP	2.5
1	A	175	PHE	2.5
1	A	280	ASN	2.5
1	A	667	ALA	2.4
1	A	969	PHE	2.4
2	B	47	G	2.4
3	C	5	DA	2.4
1	A	1041	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	288	ASP	2.4
1	A	988	ILE	2.4
1	A	237	SER	2.4
1	A	970	LYS	2.4
1	A	689	PHE	2.4
1	A	10	LEU	2.4
1	A	861	LEU	2.4
1	A	54	SER	2.4
1	A	1052	PRO	2.4
1	A	325	ARG	2.4
1	A	932	PHE	2.4
1	A	279	GLU	2.4
2	B	41	U	2.4
1	A	483	GLY	2.3
1	A	735	THR	2.3
1	A	17	ALA	2.3
1	A	435	ASP	2.3
1	A	810	MET	2.3
1	A	340	LEU	2.3
1	A	787	LEU	2.3
1	A	497	GLU	2.3
1	A	468	PRO	2.3
2	B	118	A	2.3
1	A	360	ALA	2.3
1	A	90	LEU	2.3
1	A	1028	LEU	2.3
1	A	354	GLU	2.3
2	B	87	G	2.3
1	A	498	THR	2.3
1	A	972	SER	2.3
1	A	964	ASP	2.3
2	B	122	C	2.3
1	A	183	ARG	2.3
1	A	108	LEU	2.3
1	A	660	LEU	2.3
1	A	1026	LEU	2.3
1	A	410	PHE	2.3
1	A	1011	LYS	2.3
2	B	110	U	2.3
3	C	29	DA	2.3
1	A	379	PHE	2.3
4	D	10	DT	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	723	VAL	2.3
1	A	272	LEU	2.2
1	A	427	LEU	2.2
1	A	186	GLN	2.2
1	A	712	ASN	2.2
1	A	788	GLU	2.2
1	A	20	GLY	2.2
1	A	933	LEU	2.2
1	A	939	TRP	2.2
1	A	247	LYS	2.2
1	A	925	PHE	2.2
1	A	1049	LYS	2.2
1	A	722	VAL	2.2
1	A	948	ASN	2.2
1	A	222	LEU	2.2
1	A	212	PHE	2.2
1	A	816	THR	2.2
1	A	734	ILE	2.2
2	B	66	A	2.2
1	A	765	THR	2.2
1	A	802	VAL	2.2
1	A	115	GLN	2.2
1	A	476	GLN	2.2
1	A	178	GLU	2.2
1	A	402	ASN	2.2
1	A	984	LYS	2.2
3	C	1	DT	2.2
1	A	309	VAL	2.1
1	A	307	SER	2.1
1	A	367	ALA	2.1
2	B	91	U	2.1
2	B	2	G	2.1
1	A	917	ALA	2.1
1	A	1020	GLU	2.1
1	A	416	LEU	2.1
1	A	425	LEU	2.1
1	A	492	ALA	2.1
4	D	9	DT	2.1
2	B	69	G	2.1
1	A	159	LEU	2.1
1	A	261	TYR	2.1
1	A	968	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	89	U	2.1
1	A	154	ASN	2.1
2	B	44	A	2.1
2	B	120	A	2.1
1	A	9	ILE	2.1
1	A	291	ARG	2.1
1	A	69	THR	2.1
2	B	4	C	2.1
1	A	44	GLU	2.1
1	A	234	PRO	2.1
1	A	83	LEU	2.0
1	A	242	LEU	2.0
1	A	429	GLN	2.0
1	A	358	LEU	2.0
1	A	424	LEU	2.0
1	A	670	LEU	2.0
1	A	299	TYR	2.0
1	A	1021	GLY	2.0
1	A	784	LYS	2.0
1	A	1031	GLU	2.0
1	A	304	LEU	2.0
1	A	312	ILE	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.