

# Full wwPDB X-ray Structure Validation Report (i)

### Jul 10, 2023 – 12:15 PM JST

PDB ID	:	8HNW
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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
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)	:	2.34

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

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.



Matria	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# \text{Entries, resolution range}(\text{\AA}))$
R <sub>free</sub>	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)
RNA backbone	3102	1012 (3.88-2.96)

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	А	1055	4% 57%	19%	23%			
2	В	128	31% 34%	47%	• 16%			
3	С	35	43%	57%				
4	D	11	18%					



#### 8HNW

# 2 Entry composition (i)

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	А	809	Total 6071	C 3867	N 1084	O 1100	S 20	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

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

• Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	107	Total 2251	C 1010	N 380	О 754	Р 107	0	0	0

• Molecule 3 is a DNA chain called Target strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	35	Total	С	Ν	0	Р	0	0	0
		00	721	347	133	207	34		0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	D	11	Total 223	C 110	N 37	O 66	Р 10	0	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: CRISPR-associated endonuclease Cas9







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	158.87Å 185.76Å 160.88Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	44.62 - 3.41	Depositor
Resolution (A)	49.01 - 3.41	EDS
% Data completeness	73.6(44.62-3.41)	Depositor
(in resolution range)	$74.1 \ (49.01 - 3.41)$	EDS
$R_{merge}$	0.13	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.78 (at 3.40 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
B B.	0.258 , $0.281$	Depositor
$n, n_{free}$	0.257 , $0.279$	DCC
$R_{free}$ test set	1185 reflections $(4.88\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	39.6	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.26 , $52.4$	EDS
L-test for $twinning^2$	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.74	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.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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).

Mal	Chain	Bond	lengths	Bond angles		
WIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.25	0/6172	0.51	1/8365~(0.0%)	
2	В	0.20	0/2508	0.81	0/3891	
3	С	0.53	0/810	0.95	0/1250	
4	D	0.52	0/249	1.04	0/383	
All	All	0.28	0/9739	0.67	1/13889~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
1	А	791	LEU	CA-CB-CG	5.81	128.66	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	6071	0	5880	140	0
2	В	2251	0	1146	56	0
3	С	721	0	399	20	0
4	D	223	0	129	0	0
All	All	9266	0	7554	197	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.



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	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:926:THR:HG1	1:A:968:THR:HG1	1.44	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

All (197) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



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



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:124:LEU:O	1:A:229:LEU:HD13	2.12	0.49
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



	boue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:973:LEU:HD11	1:A:1030:PHE:CE2	2.51	0.46
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:HG22	1:A:441:ILE:O	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:1001:ASN:ND2	3:C:5:DA:N7	2.66	0.43
2:B:120:A:HO2'	2:B:121:U:H6	1.63	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



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:10:LEU:HG	1:A:491:PRO:HG2	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
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: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: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 (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	А	788/1055~(75%)	731 (93%)	57 (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	А	593/918~(65%)	587~(99%)	6 (1%)	76 88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	208	ARG
1	А	216	PHE
1	А	254	TYR
1	А	284	ARG
1	А	356	ASN
1	А	665	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	368	ASN
1	А	430	GLN



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$\mathbf{Mol}$	Chain	$\mathbf{Res}$	Type
1	А	467	ASN

#### 5.3.3 RNA (i)

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

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	В	43	G
2	В	44	А
2	В	65	А
2	В	88	С
2	В	117	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	В	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 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

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	А	809/1055~(76%)	0.28	43 (5%) 26 28	5, 58, 99, 129	0
2	В	107/128~(83%)	1.79	40 (37%) 0 0	7, 56, 159, 190	0
3	С	35/35~(100%)	0.99	7 (20%) 1 1	13, 44, 80, 83	0
4	D	11/11 (100%)	1.07	2 (18%) 1 2	25, 29, 75, 76	0
All	All	962/1229~(78%)	0.48	92 (9%) 8 10	5, 57, 105, 190	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	115	G	6.2
2	В	97	U	6.0
2	В	43	G	5.8
2	В	117	G	5.8
1	А	22	ALA	5.4
2	В	110	U	5.2
2	В	116	G	5.2
2	В	42	С	5.1
1	А	719	ASP	4.9
2	В	70	А	4.7
4	D	11	DA	4.6
2	В	90	С	4.5
1	А	1045	CYS	4.4
2	В	94	С	4.4
1	А	289	ASN	4.4
4	D	10	DT	4.3
2	В	47	G	4.2
2	В	113	A	4.2
2	В	80	U	4.1
1	А	31	ASN	4.0
1	А	32	PRO	3.9



Mol	Chain	Res	Type	RSRZ
2	В	98	U	3.9
1	А	792	PRO	3.8
2	В	40	U	3.8
2	В	79	С	3.8
1	А	388	ILE	3.6
1	А	695	ILE	3.6
1	А	153	ASP	3.4
1	А	356	ASN	3.4
1	А	783	PRO	3.4
1	А	246	GLY	3.4
1	А	144	GLU	3.3
1	А	791	LEU	3.3
2	В	119	С	3.3
3	С	4	DA	3.3
2	В	95	С	3.3
2	В	48	А	3.2
1	А	1034	GLN	3.1
1	А	393	ALA	3.1
2	В	1	G	3.1
1	А	357	ASN	3.1
2	В	118	А	3.1
1	А	780	SER	3.1
3	С	30	DG	3.0
1	А	806	PHE	3.0
1	А	726	SER	2.9
2	В	88	С	2.9
2	В	112	С	2.9
2	В	122	С	2.9
2	В	41	U	2.9
2	В	2	G	2.9
2	В	114	A	2.9
2	В	120	А	2.9
3	С	5	DA	2.8
1	А	661	ASN	2.8
2	В	92	G	2.8
1	А	782	ASN	2.8
2	В	46	A	2.7
2	В	12	С	2.7
1	А	431	GLY	2.6
1	А	392	LEU	2.6
2	В	44	А	2.6
1	А	785	LEU	2.6



Mol	Chain	$\operatorname{Res}$	Type	RSRZ
2	В	126	U	2.5
1	А	676	ASP	2.5
1	А	790	ARG	2.5
2	В	111	U	2.5
3	С	31	DT	2.5
1	А	772	GLN	2.5
1	А	964	ASP	2.5
1	А	1048	SER	2.5
2	В	69	G	2.4
2	В	89	U	2.4
1	А	801	PHE	2.4
3	С	3	DA	2.4
1	А	959	ASP	2.3
1	А	376	GLY	2.3
1	А	770	PHE	2.3
1	А	774	VAL	2.3
1	А	436	GLU	2.3
3	С	1	DT	2.2
1	А	948	ASN	2.2
3	С	8	DA	2.2
1	А	280	ASN	2.2
2	В	3	U	2.2
1	А	1047	PRO	2.2
1	А	109	ASP	2.1
1	А	85	SER	2.1
2	В	78	U	2.1
2	В	96	С	2.1
2	В	49	А	2.0
1	А	136	ASN	2.0

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## 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.

