



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 10, 2023 – 12:10 PM JST

PDB ID : 8HNT
Title : Crystal structure of anti-CRISPR protein AcrIIC4 bound to HpaCas9-sgRNA surveillance complex
Authors : Sun, W.; Cheng, Z.; Wang, Y.
Deposited on : 2022-12-08
Resolution : 3.06 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
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

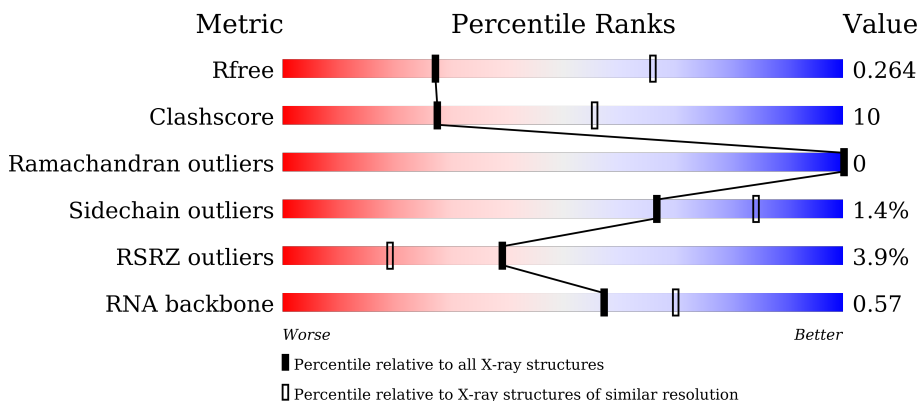
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)
RNA backbone	3102	1036 (3.32-2.80)

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	 4% 70% 24% 5%
2	B	128	 5% 49% 23% 7% 20%
3	C	89	 78% 21% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10612 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
			Total	C	N	O	S			
1	A	1000	7795	4961	1411	1403	20	0	0	0

There is a discrepancy between the modelled and reference sequences:

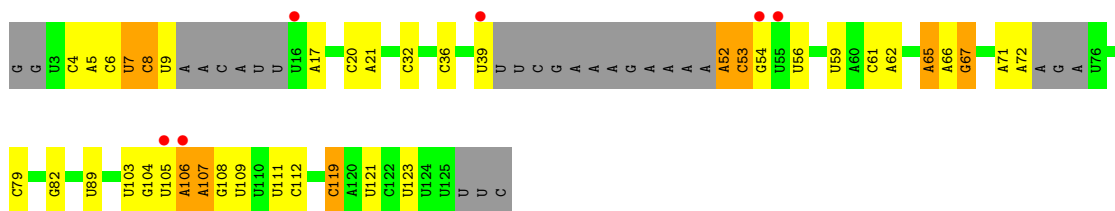
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP F0ET08

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	102	2144	962	359	721	102	0	0	0

- Molecule 3 is a protein called anti-CRISPR protein AcrIIC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	88	673	431	114	127	1	0	0	0



● Molecule 3: anti-CRISPR protein AcrIIC4

Chain C: 78% 21%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	205.83Å 134.59Å 67.53Å 90.00° 105.04° 90.00°	Depositor
Resolution (Å)	33.22 – 3.06 50.13 – 3.06	Depositor EDS
% Data completeness (in resolution range)	78.4 (33.22-3.06) 78.5 (50.13-3.06)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 3.07Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.237 , 0.264 0.236 , 0.264	Depositor DCC
R_{free} test set	1386 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtrriage
Anisotropy	0.365	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	10612	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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	0.25	0/7939	0.51	1/10731 (0.0%)
2	B	0.18	0/2388	0.79	0/3704
3	C	0.25	0/684	0.44	0/919
All	All	0.24	0/11011	0.59	1/15354 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	760	PRO	N-CA-CB	5.91	110.39	103.30

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	A	7795	0	7672	179	0
2	B	2144	0	1091	21	0
3	C	673	0	662	12	0
All	All	10612	0	9425	199	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 10.

All (199) 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:593:PHE:O	1:A:641:LYS:NZ	2.24	0.71
1:A:982:VAL:HG12	1:A:1029:SER:HB2	1.74	0.70
1:A:382:TYR:HB2	1:A:388:ILE:HG22	1.77	0.67
1:A:496:ILE:HD13	1:A:670:LEU:HD23	1.77	0.67
1:A:700:ARG:HG2	1:A:706:ALA:HA	1.78	0.66
1:A:585:PHE:HB3	1:A:738:VAL:HG11	1.77	0.66
1:A:829:ARG:HB3	1:A:834:ILE:HG13	1.77	0.66
1:A:71:ARG:HH12	2:B:20:C:H5'	1.60	0.65
1:A:343:MET:HB3	1:A:346:TYR:HB3	1.79	0.65
1:A:277:ILE:HD13	1:A:315:LEU:HD11	1.76	0.65
1:A:705:LEU:HD13	1:A:718:LEU:HD22	1.78	0.64
1:A:78:LYS:HD3	1:A:228:LEU:HD21	1.79	0.64
1:A:47:GLU:OE2	1:A:509:ARG:NH2	2.29	0.64
1:A:38:VAL:HG13	1:A:805:LEU:HD12	1.79	0.64
1:A:414:ILE:HG23	1:A:416:LEU:H	1.61	0.64
1:A:700:ARG:HG3	1:A:705:LEU:HD12	1.79	0.63
1:A:701:SER:HA	1:A:706:ALA:HB2	1.81	0.62
1:A:353:LEU:HD21	1:A:400:VAL:HG13	1.80	0.62
1:A:555:GLN:HE22	1:A:598:LEU:HB3	1.65	0.61
1:A:275:LEU:HD23	1:A:286:LEU:HD11	1.82	0.61
1:A:715:HIS:O	1:A:718:LEU:HB2	1.99	0.61
1:A:825:LYS:HG2	1:A:835:SER:OG	2.00	0.60
1:A:478:ARG:HE	1:A:482:ASN:HD21	1.47	0.60
1:A:275:LEU:HD11	1:A:321:PHE:HD2	1.64	0.60
1:A:9:ILE:HG13	1:A:26:ILE:HD13	1.83	0.60
1:A:555:GLN:NE2	1:A:598:LEU:HB3	2.17	0.60
1:A:290:GLU:HB3	1:A:313:LEU:HD22	1.84	0.59
1:A:835:SER:HB2	1:A:901:GLN:HB2	1.84	0.59
1:A:943:LYS:NZ	2:B:67:G:OP1	2.34	0.59
1:A:266:PHE:O	1:A:270:THR:HG23	2.03	0.59
1:A:273:ASN:OD1	1:A:291:ARG:NH2	2.36	0.58
1:A:271:LYS:HD3	1:A:341:MET:HG2	1.85	0.58
1:A:594:ASN:HA	1:A:641:LYS:HG3	1.85	0.57
1:A:923:ASP:HB3	1:A:925:PHE:HE1	1.68	0.57
1:A:306:TYR:HA	1:A:309:VAL:HG12	1.85	0.57
1:A:9:ILE:HG12	1:A:493:ARG:HB2	1.87	0.56
1:A:826:SER:HB3	1:A:836:VAL:HG13	1.86	0.56
1:A:895:VAL:HG23	2:B:56:U:H5'	1.87	0.56
1:A:297:GLN:HB2	1:A:304:LEU:HD13	1.87	0.56
1:A:821:MET:HG3	1:A:915:ASP:HB2	1.87	0.56
1:A:271:LYS:HE2	1:A:340:LEU:O	2.06	0.56
2:B:103:U:H3'	2:B:104:G:H8	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:MET:HB2	1:A:347:HIS:HD2	1.71	0.55
1:A:294:LEU:HD11	1:A:309:VAL:HG23	1.88	0.55
1:A:336:THR:HG22	1:A:337:LYS:HD2	1.88	0.55
1:A:255:LYS:NZ	3:C:15:GLU:OE2	2.28	0.55
1:A:551:LEU:O	1:A:555:GLN:HG3	2.07	0.55
1:A:767:TRP:NE1	1:A:773:GLU:OE1	2.40	0.55
1:A:603:GLU:N	1:A:603:GLU:OE1	2.40	0.55
1:A:897:VAL:HG22	1:A:898:GLU:H	1.70	0.55
1:A:942:ALA:O	1:A:1054:ARG:NH1	2.40	0.55
1:A:83:LEU:HD22	1:A:88:ILE:HD12	1.89	0.54
1:A:343:MET:HB2	1:A:347:HIS:CD2	2.42	0.54
1:A:90:LEU:HD23	1:A:90:LEU:H	1.72	0.53
1:A:641:LYS:O	1:A:645:ILE:HG12	2.08	0.53
1:A:167:PRO:HD2	1:A:201:GLU:HB2	1.89	0.53
1:A:8:TYR:CD2	1:A:23:VAL:HG13	2.44	0.53
1:A:571:LEU:HD12	1:A:577:VAL:HG21	1.90	0.52
1:A:370:THR:O	1:A:374:GLU:HG3	2.10	0.52
1:A:349:ILE:HA	1:A:352:VAL:HG22	1.91	0.52
3:C:38:ALA:HB2	3:C:73:LYS:HB2	1.91	0.52
1:A:10:LEU:HD12	1:A:484:VAL:HG11	1.92	0.52
1:A:866:LYS:O	1:A:870:GLU:HG2	2.09	0.52
1:A:908:ARG:NH2	2:B:65:A:O2'	2.42	0.52
2:B:52:A:O2'	2:B:53:C:OP1	2.23	0.52
1:A:478:ARG:HE	1:A:482:ASN:ND2	2.09	0.51
1:A:96:LEU:HD23	1:A:119:ALA:HA	1.92	0.51
1:A:52:GLY:HA3	1:A:506:TYR:CD2	2.46	0.51
1:A:857:ARG:O	2:B:36:C:H4'	2.12	0.50
1:A:110:HIS:O	1:A:209:GLN:NE2	2.44	0.50
2:B:103:U:H3'	2:B:104:G:C8	2.46	0.50
1:A:382:TYR:HE1	3:C:6:SER:HA	1.76	0.50
1:A:298:PRO:O	1:A:347:HIS:NE2	2.34	0.50
1:A:505:SER:O	1:A:509:ARG:HG3	2.12	0.50
1:A:825:LYS:HB2	1:A:913:VAL:HG13	1.93	0.50
1:A:106:GLU:O	1:A:110:HIS:HB3	2.12	0.50
1:A:650:LEU:HD23	1:A:651:ASP:H	1.77	0.50
1:A:222:LEU:O	1:A:226:THR:HG23	2.11	0.50
1:A:427:LEU:HB3	1:A:432:LEU:HD12	1.94	0.50
1:A:454:HIS:ND1	1:A:679:HIS:HB2	2.26	0.49
1:A:501:GLU:HB2	1:A:509:ARG:HD2	1.93	0.49
3:C:74:LEU:HD23	3:C:78:ILE:HG12	1.94	0.49
2:B:66:A:N6	2:B:82:G:O2'	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:U:OP1	3:C:28:ARG:NH2	2.43	0.49
1:A:857:ARG:HG2	2:B:54:G:H21	1.78	0.48
2:B:106:A:H5'	2:B:107:A:C5	2.48	0.48
1:A:291:ARG:HH22	1:A:431:GLY:HA2	1.76	0.48
1:A:46:ALA:HB3	1:A:469:VAL:HA	1.94	0.48
1:A:347:HIS:HB3	1:A:350:ARG:HH21	1.79	0.48
1:A:836:VAL:HA	1:A:897:VAL:O	2.14	0.48
1:A:104:ARG:NH2	1:A:201:GLU:OE2	2.40	0.48
1:A:277:ILE:O	1:A:283:GLU:HA	2.14	0.47
1:A:16:ILE:HD12	1:A:45:ARG:HD2	1.95	0.47
1:A:970:LYS:HD3	1:A:970:LYS:HA	1.63	0.47
1:A:100:VAL:HG21	1:A:123:HIS:CD2	2.49	0.47
1:A:350:ARG:HB2	1:A:365:LEU:HD13	1.97	0.47
1:A:428:MET:HA	1:A:432:LEU:HB2	1.96	0.47
1:A:982:VAL:HG23	1:A:987:THR:OG1	2.14	0.47
1:A:310:ARG:NH1	1:A:319:ALA:O	2.38	0.47
1:A:199:LEU:HD11	1:A:226:THR:HG22	1.97	0.47
1:A:1005:LYS:HG3	1:A:1009:LEU:HD21	1.97	0.47
1:A:714:ARG:HH21	1:A:1007:HIS:CE1	2.32	0.47
1:A:520:ARG:O	1:A:523:ARG:HG3	2.14	0.46
1:A:169:GLU:HA	1:A:172:VAL:HG22	1.97	0.46
1:A:298:PRO:HG3	1:A:304:LEU:HD22	1.96	0.46
1:A:310:ARG:NE	1:A:335:GLU:OE2	2.44	0.46
1:A:799:HIS:CE1	1:A:801:PHE:HB2	2.49	0.46
1:A:772:GLN:O	1:A:776:ILE:HG12	2.14	0.46
1:A:1035:VAL:HG22	1:A:1042:ILE:HG13	1.97	0.46
1:A:111:LYS:HA	1:A:209:GLN:HE22	1.81	0.46
1:A:844:LEU:HD21	1:A:849:LEU:HB2	1.96	0.46
1:A:924:VAL:HG22	1:A:933:LEU:HD22	1.98	0.46
1:A:652:GLU:O	1:A:656:ILE:HG13	2.15	0.46
1:A:302:ASN:HA	1:A:347:HIS:CE1	2.51	0.45
2:B:61:C:H2'	2:B:62:A:H8	1.80	0.45
1:A:103:LEU:O	1:A:107:GLY:N	2.45	0.45
1:A:294:LEU:HD11	1:A:313:LEU:HD11	1.97	0.45
3:C:60:GLU:O	3:C:64:LYS:HG2	2.16	0.45
1:A:128:ARG:O	1:A:195:ARG:HD3	2.17	0.45
1:A:738:VAL:HA	1:A:741:GLU:HG2	1.99	0.45
1:A:827:ALA:HB2	1:A:913:VAL:HB	1.98	0.45
1:A:255:LYS:HD2	1:A:255:LYS:H	1.82	0.45
1:A:932:PHE:O	1:A:933:LEU:HD23	2.17	0.45
1:A:275:LEU:HD11	1:A:321:PHE:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:LYS:HA	1:A:1046:LYS:HD2	1.78	0.44
1:A:261:TYR:HE1	1:A:299:TYR:HE2	1.65	0.44
1:A:530:PHE:CE2	1:A:541:PRO:HB3	2.53	0.44
1:A:628:PHE:O	1:A:632:VAL:HG12	2.17	0.44
1:A:719:ASP:O	1:A:722:VAL:HG22	2.18	0.44
1:A:1035:VAL:HG12	1:A:1036:ASP:O	2.18	0.44
1:A:814:LYS:HE2	1:A:814:LYS:HB3	1.60	0.44
1:A:497:GLU:OE2	1:A:693:GLY:HA2	2.17	0.44
1:A:671:CYS:HA	1:A:688:VAL:HG11	1.98	0.44
1:A:512:LEU:HD23	1:A:512:LEU:O	2.18	0.44
1:A:512:LEU:HD23	1:A:516:GLN:HG3	1.99	0.44
1:A:700:ARG:NH1	1:A:719:ASP:OD1	2.51	0.44
1:A:148:LEU:HD12	1:A:189:TYR:CE1	2.52	0.43
1:A:680:LEU:HB2	1:A:687:LYS:HD2	2.00	0.43
2:B:111:U:H2'	2:B:112:C:C6	2.53	0.43
1:A:261:TYR:CD2	1:A:369:PRO:HB3	2.53	0.43
1:A:46:ALA:HB2	1:A:472:ARG:HD2	2.01	0.43
1:A:375:ILE:HA	1:A:392:LEU:HD11	2.01	0.43
1:A:900:ILE:HG23	1:A:902:LYS:HE3	2.00	0.43
1:A:560:LEU:HB3	1:A:628:PHE:HE1	1.83	0.43
1:A:925:PHE:CE1	1:A:969:PHE:HD1	2.36	0.43
1:A:177:VAL:HG13	1:A:178:GLU:HG3	2.00	0.43
1:A:550:ARG:HD3	1:A:593:PHE:CZ	2.53	0.43
1:A:43:PHE:CD2	1:A:476:GLN:HG3	2.53	0.43
1:A:260:THR:HG22	1:A:376:GLY:HA3	1.99	0.43
1:A:965:ASN:OD1	1:A:965:ASN:N	2.50	0.43
1:A:577:VAL:HB	1:A:598:LEU:HD11	2.00	0.43
1:A:206:PHE:HZ	1:A:225:LEU:HD12	1.84	0.42
1:A:852:MET:SD	1:A:854:ASN:HB2	2.59	0.42
1:A:897:VAL:HG22	1:A:898:GLU:N	2.34	0.42
1:A:482:ASN:O	1:A:486:ARG:HG3	2.19	0.42
1:A:647:SER:O	1:A:648:GLN:HB2	2.20	0.42
1:A:307:SER:HB2	1:A:336:THR:HA	2.02	0.42
1:A:461:PRO:HB2	1:A:464:GLU:HG3	2.01	0.42
1:A:813:ARG:HD2	2:B:119:C:O2'	2.19	0.42
1:A:637:PHE:CG	1:A:641:LYS:HD3	2.54	0.42
1:A:820:HIS:CD2	1:A:907:VAL:HG11	2.55	0.42
1:A:353:LEU:HD23	1:A:353:LEU:HA	1.87	0.42
3:C:61:LYS:HG2	3:C:65:GLU:OE2	2.20	0.42
1:A:344:LYS:O	1:A:348:GLN:HB2	2.20	0.42
1:A:493:ARG:HH11	1:A:687:LYS:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:LYS:HB2	1:A:989:LEU:HD13	2.02	0.42
1:A:82:LEU:HD11	1:A:224:ASN:HB3	2.02	0.41
1:A:259:ASN:HB3	1:A:345:ALA:HB2	2.00	0.41
1:A:594:ASN:HB2	1:A:644:ARG:NH1	2.35	0.41
1:A:854:ASN:O	1:A:858:GLU:N	2.41	0.41
1:A:271:LYS:CD	1:A:341:MET:HG2	2.50	0.41
1:A:576:TYR:CD2	1:A:577:VAL:HG13	2.55	0.41
3:C:29:GLU:HB2	3:C:30:PRO:HD3	2.02	0.41
1:A:100:VAL:HA	1:A:103:LEU:HB2	2.02	0.41
1:A:552:TYR:CZ	1:A:568:LEU:HB2	2.56	0.41
1:A:583:LEU:HB3	1:A:588:THR:HG21	2.01	0.41
1:A:908:ARG:O	1:A:909:GLU:HG2	2.21	0.41
3:C:23:LEU:HD21	3:C:86:ILE:HD11	2.03	0.41
1:A:718:LEU:HD23	1:A:778:ILE:HD12	2.02	0.41
1:A:727:THR:O	1:A:731:GLN:HG3	2.20	0.41
2:B:7:U:HO2'	2:B:8:C:P	2.44	0.41
1:A:27:ASP:HB3	1:A:33:LEU:HD21	2.03	0.41
1:A:555:GLN:OE1	1:A:560:LEU:HD13	2.21	0.41
1:A:695:ILE:HD13	1:A:695:ILE:HA	1.85	0.41
3:C:74:LEU:HD23	3:C:74:LEU:O	2.20	0.41
1:A:73:VAL:HG12	1:A:77:LYS:HE3	2.03	0.41
1:A:631:LEU:O	1:A:634:THR:HG22	2.20	0.41
2:B:53:C:H2'	2:B:54:G:O4'	2.20	0.40
1:A:89:LEU:HG	1:A:91:SER:O	2.21	0.40
1:A:98:HIS:O	2:B:59:U:O2'	2.34	0.40
1:A:720:ALA:O	1:A:723:VAL:HG12	2.21	0.40
1:A:959:ASP:OD1	1:A:959:ASP:N	2.53	0.40
2:B:71:A:H4'	3:C:80:LEU:CD2	2.51	0.40
1:A:650:LEU:HG	1:A:652:GLU:HG3	2.04	0.40
1:A:844:LEU:O	1:A:876:PRO:HB3	2.21	0.40
1:A:857:ARG:HG2	2:B:54:G:N2	2.36	0.40
2:B:61:C:H2'	2:B:62:A:C8	2.56	0.40
3:C:81:ALA:HB3	3:C:88:PHE:HE2	1.86	0.40
1:A:302:ASN:HA	1:A:347:HIS:NE2	2.36	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	A	984/1055 (93%)	940 (96%)	44 (4%)	0	100	100
3	C	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
All	All	1070/1144 (94%)	1024 (96%)	46 (4%)	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	787/919 (86%)	776 (99%)	11 (1%)	67	84
3	C	69/77 (90%)	68 (99%)	1 (1%)	67	84
All	All	856/996 (86%)	844 (99%)	12 (1%)	67	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	208	ARG
1	A	318	GLU
1	A	478	ARG
1	A	520	ARG
1	A	522	GLN
1	A	523	ARG
1	A	574	LYS

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Mol	Chain	Res	Type
1	A	655	PHE
1	A	828	LYS
1	A	993	ASN
3	C	8	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	555	GLN
1	A	993	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	99/128 (77%)	23 (23%)	2 (2%)

All (23) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	4	C
2	B	5	A
2	B	6	C
2	B	7	U
2	B	8	C
2	B	9	U
2	B	17	A
2	B	21	A
2	B	32	C
2	B	39	U
2	B	53	C
2	B	65	A
2	B	67	G
2	B	72	A
2	B	79	C
2	B	89	U
2	B	105	U
2	B	106	A
2	B	107	A
2	B	108	G
2	B	109	U

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Mol	Chain	Res	Type
2	B	119	C
2	B	121	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	7	U
2	B	52	A

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, 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	1000/1055 (94%)	0.09	40 (4%) 38 18	23, 60, 111, 126	0
2	B	102/128 (79%)	0.50	6 (5%) 22 9	30, 61, 123, 171	0
3	C	88/89 (98%)	-0.13	0 100 100	35, 55, 71, 77	0
All	All	1190/1272 (93%)	0.11	46 (3%) 39 19	23, 59, 112, 171	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	LEU	4.4
1	A	311	SER	4.4
2	B	105	U	4.3
1	A	854	ASN	4.3
1	A	269	ILE	4.2
1	A	374	GLU	4.2
1	A	272	LEU	4.2
1	A	266	PHE	4.1
1	A	265	ARG	3.7
1	A	345	ALA	3.4
1	A	315	LEU	3.4
1	A	249	THR	3.2
1	A	423	LYS	3.2
1	A	275	LEU	3.0
1	A	299	TYR	3.0
1	A	422	TYR	3.0
1	A	346	TYR	3.0
1	A	330	ASP	2.8
1	A	349	ILE	2.8
2	B	106	A	2.7
1	A	268	TRP	2.7
1	A	873	ASN	2.7
2	B	39	U	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	453	ASN	2.6
1	A	321	PHE	2.6
1	A	295	MET	2.6
1	A	263	ALA	2.6
1	A	270	THR	2.5
1	A	370	THR	2.5
1	A	371	LEU	2.5
1	A	441	ILE	2.5
1	A	363	ALA	2.4
2	B	54	G	2.4
1	A	261	TYR	2.4
1	A	434	TYR	2.4
1	A	352	VAL	2.3
1	A	277	ILE	2.3
1	A	390	ALA	2.3
1	A	391	TYR	2.3
1	A	424	LEU	2.3
1	A	309	VAL	2.3
1	A	392	LEU	2.2
2	B	55	U	2.2
1	A	393	ALA	2.1
2	B	16	U	2.1
1	A	898	GLU	2.1

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.