



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2017 – 01:27 PM EDT

PDB ID : 5U34
Title : Crystal structure of AacC2c1-sgRNA binary complex
Authors : Yang, H.; Gao, P.; Rajashankar, K.R.; Patel, D.J.
Deposited on : unknown
Resolution : 3.25 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

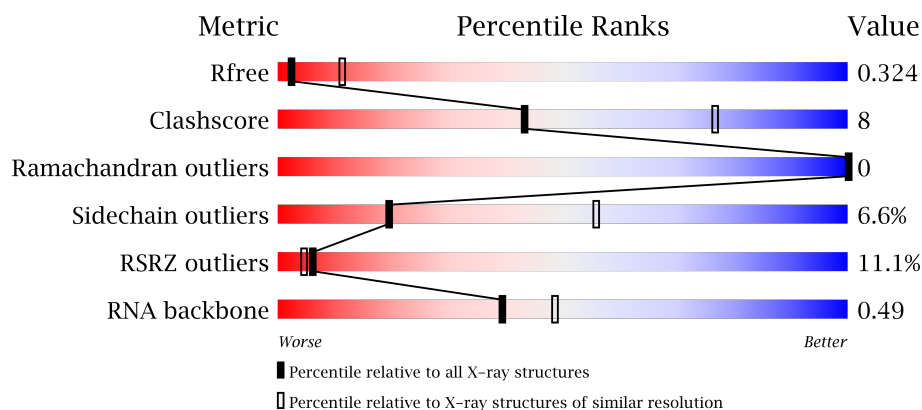
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	100719	1852 (3.32-3.20)
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)
RNA backbone	2435	1085 (3.72-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1130	<div> <div>10%</div> <div>65%</div> <div>18%</div> <div>•</div> <div>15%</div> </div>
2	B	112	<div> <div>3%</div> <div>33%</div> <div>35%</div> <div>•</div> <div>30%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9562 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 C2c1.

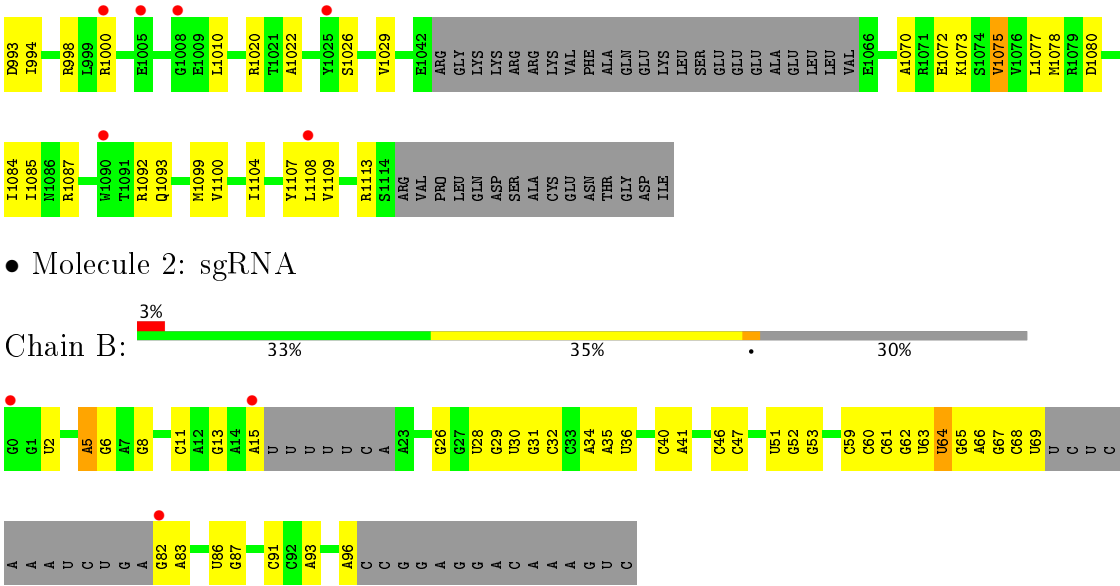
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	960	Total	C	N	O	S	Se	0	0	0
			7882	4978	1458	1420	8	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP T0D7A2
A	848	ALA	GLU	engineered mutation	UNP T0D7A2

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	P	0	0	0
			1680	749	315	538	78			



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.47Å 128.20Å 155.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.33 – 3.25 73.58 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.33-3.25) 98.6 (73.58-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 3.26Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.270 , 0.324 0.268 , 0.324	Depositor DCC
R_{free} test set	1303 reflections (4.90%)	DCC
Wilson B-factor (Å ²)	112.4	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9562	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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	0.23	0/8030	0.38	0/10784
2	B	0.36	2/1880 (0.1%)	0.80	5/2927 (0.2%)
All	All	0.26	2/9910 (0.0%)	0.50	5/13711 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	30	U	C4-O4	12.96	1.34	1.23
2	B	30	U	N3-C4	-5.16	1.33	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	30	U	N3-C4-C5	12.02	121.81	114.60
2	B	30	U	C2-N3-C4	-11.39	120.17	127.00
2	B	30	U	C5-C4-O4	-9.54	120.18	125.90
2	B	30	U	N1-C2-N3	7.29	119.27	114.90
2	B	30	U	N1-C2-O2	-5.19	119.17	122.80

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	7882	0	7809	125	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1680	0	848	12	0
All	All	9562	0	8657	132	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 8.

All (132) 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:859:ARG:HG3	1:A:861:PRO:HD2	1.67	0.76
1:A:12:LEU:HD23	1:A:15:MSE:HE3	1.72	0.70
1:A:1022:ALA:O	1:A:1026:SER:OG	2.09	0.70
1:A:859:ARG:HG2	1:A:956:GLU:HB3	1.74	0.68
1:A:245:LEU:HB3	1:A:371:LEU:HD23	1.75	0.68
1:A:913:ARG:HB3	1:A:958:GLU:H	1.59	0.68
1:A:419:ARG:NH2	1:A:436:ASP:OD2	2.28	0.67
1:A:860:PRO:O	1:A:864:ASN:N	2.27	0.67
1:A:419:ARG:HB3	1:A:438:THR:HG22	1.77	0.66
1:A:859:ARG:HD2	1:A:860:PRO:HD2	1.76	0.66
1:A:407:LEU:HB3	1:A:410:GLU:HG3	1.77	0.66
1:A:963:PRO:HD3	1:A:1104:ILE:HD11	1.76	0.66
1:A:859:ARG:HH11	1:A:860:PRO:HD2	1.61	0.65
1:A:894:TYR:O	1:A:987:ARG:NH2	2.29	0.63
1:A:226:GLU:OE2	1:A:393:ARG:NH1	2.31	0.63
1:A:400:ASN:N	1:A:400:ASN:OD1	2.32	0.62
1:A:213:VAL:O	1:A:218:ARG:NH1	2.32	0.62
1:A:543:SER:OG	1:A:586:ARG:NH2	2.32	0.61
1:A:637:GLU:HG2	1:A:640:ARG:HH12	1.66	0.60
1:A:566:VAL:HG22	1:A:844:LEU:HB3	1.84	0.59
1:A:73:LEU:HG	1:A:95:LEU:HD23	1.84	0.58
1:A:731:ARG:HD3	2:B:47:C:H5"	1.85	0.58
1:A:998:ARG:HG3	1:A:1078:MSE:HE2	1.87	0.57
1:A:574:ARG:NH2	1:A:956:GLU:OE1	2.37	0.56
1:A:939:HIS:HD2	1:A:1109:VAL:HG11	1.70	0.56
1:A:764:LEU:HB3	1:A:801:ILE:HG12	1.88	0.56
1:A:77:ARG:NH2	1:A:90:GLY:O	2.38	0.55
1:A:205:LYS:O	1:A:214:ARG:NH1	2.41	0.54
1:A:573:LEU:HD13	1:A:868:MSE:HE1	1.89	0.54
1:A:264:VAL:O	1:A:268:ASN:ND2	2.41	0.53
1:A:939:HIS:O	1:A:1113:ARG:NH2	2.26	0.53
1:A:105:LEU:HD21	1:A:175:THR:HA	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:VAL:HG21	1:A:1092:ARG:HH11	1.74	0.53
1:A:914:ARG:HH22	2:B:2:U:H1'	1.72	0.53
1:A:1085:ILE:HG13	1:A:1100:VAL:HG22	1.92	0.52
1:A:43:LEU:HD23	1:A:72:LEU:HD11	1.91	0.52
1:A:4:LYS:HE2	1:A:885:VAL:HG21	1.91	0.52
1:A:1108:LEU:HD12	1:A:1109:VAL:HG23	1.92	0.52
1:A:648:GLN:OE1	1:A:685:THR:OG1	2.24	0.52
1:A:76:LEU:HD22	1:A:95:LEU:HG	1.92	0.52
1:A:1:MSE:HE3	1:A:507:ARG:HB3	1.92	0.51
1:A:731:ARG:NH1	2:B:47:C:OP1	2.44	0.51
1:A:579:ILE:HD13	1:A:620:LEU:HD11	1.92	0.51
1:A:305:LYS:NZ	1:A:321:GLU:OE1	2.29	0.51
1:A:666:ARG:O	1:A:670:TRP:HB2	2.10	0.50
1:A:635:ARG:HA	1:A:638:ARG:HD3	1.93	0.50
1:A:904:ARG:NH2	2:B:5:A:OP2	2.44	0.50
2:B:51:U:H2'	2:B:52:G:C8	2.47	0.49
1:A:665:ARG:O	1:A:669:SER:OG	2.19	0.49
1:A:425:LYS:HD2	1:A:434:VAL:HG11	1.94	0.49
1:A:607:ASN:N	1:A:607:ASN:OD1	2.46	0.49
1:A:569:VAL:HG22	1:A:579:ILE:HG22	1.95	0.48
1:A:6:ILE:HD12	1:A:450:LEU:HD11	1.96	0.48
1:A:313:ALA:HB1	1:A:317:LEU:HD12	1.96	0.48
1:A:5:SER:HA	1:A:505:SER:HA	1.96	0.48
1:A:79:ARG:HH12	1:A:192:ARG:HE	1.61	0.47
1:A:582:PHE:HB2	1:A:985:GLN:NE2	2.29	0.47
1:A:939:HIS:CD2	1:A:1109:VAL:HG11	2.50	0.47
1:A:15:MSE:SE	1:A:18:ILE:HD12	2.64	0.47
1:A:565:ARG:HB2	1:A:842:CYS:HA	1.97	0.47
1:A:696:LEU:O	1:A:700:LYS:HG3	2.14	0.47
1:A:263:LEU:HB3	1:A:357:PHE:CZ	2.49	0.47
1:A:805:LYS:HB3	1:A:870:TRP:CZ2	2.50	0.47
1:A:125:LEU:O	1:A:129:ALA:N	2.46	0.47
1:A:85:HIS:CG	1:A:186:GLY:HA3	2.50	0.47
1:A:1078:MSE:HE3	1:A:1093:GLN:HG3	1.96	0.46
1:A:653:ARG:HH22	1:A:773:SER:HB2	1.80	0.46
1:A:915:VAL:HG11	1:A:952:ILE:HD12	1.97	0.46
1:A:454:ASP:HB3	1:A:457:GLU:HB2	1.98	0.46
1:A:314:PRO:HG2	1:A:317:LEU:HG	1.96	0.46
1:A:849:GLU:HB3	1:A:894:TYR:HA	1.96	0.46
1:A:125:LEU:HD23	1:A:218:ARG:HG2	1.96	0.46
1:A:425:LYS:HE3	1:A:434:VAL:HG21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD23	1:A:207:LEU:H	1.81	0.46
1:A:993:ASP:HB2	1:A:1020:ARG:HD3	1.97	0.45
1:A:540:ASP:N	1:A:540:ASP:OD1	2.48	0.45
1:A:575:THR:HG21	1:A:619:LEU:HD13	1.98	0.45
1:A:883:ALA:HB1	1:A:888:LEU:HB2	1.98	0.45
1:A:24:LYS:O	1:A:28:GLU:HG2	2.16	0.45
1:A:264:VAL:HG13	1:A:361:TYR:HE1	1.81	0.45
1:A:338:LEU:O	1:A:342:LEU:N	2.46	0.45
1:A:405:THR:HB	1:A:419:ARG:HG3	1.98	0.45
1:A:274:MSE:HE1	1:A:338:LEU:HA	1.97	0.45
1:A:464:ARG:HG2	1:A:471:HIS:ND1	2.32	0.45
1:A:720:ARG:HD3	1:A:720:ARG:HA	1.84	0.45
1:A:735:LYS:HG2	1:A:738:ARG:HH11	1.82	0.44
2:B:61:C:H2'	2:B:62:G:C8	2.53	0.44
1:A:227:ARG:HD2	1:A:390:ILE:HD11	2.00	0.44
1:A:15:MSE:HE1	1:A:440:PRO:HD2	1.98	0.44
1:A:457:GLU:C	1:A:459:ILE:H	2.21	0.44
1:A:824:VAL:HG21	1:A:838:LYS:HE2	1.99	0.44
1:A:1000:ARG:NH2	1:A:1070:ALA:O	2.42	0.44
1:A:266:LEU:HB3	1:A:350:LEU:HD21	2.00	0.44
1:A:72:LEU:O	1:A:76:LEU:N	2.51	0.44
1:A:586:ARG:HG3	1:A:610:LEU:HB3	1.99	0.44
1:A:670:TRP:HH2	1:A:700:LYS:HG2	1.83	0.44
2:B:40:C:H2'	2:B:41:A:H8	1.82	0.44
2:B:52:G:H2'	2:B:53:G:C8	2.53	0.44
1:A:79:ARG:NE	1:A:189:PRO:O	2.51	0.43
1:A:79:ARG:O	1:A:83:ASN:ND2	2.51	0.43
1:A:18:ILE:HG12	1:A:425:LYS:HE2	2.00	0.43
1:A:107:VAL:HG23	1:A:229:MSE:HG2	2.00	0.43
1:A:47:ASN:O	1:A:65:ALA:HA	2.19	0.43
2:B:40:C:H2'	2:B:41:A:C8	2.53	0.43
1:A:453:ARG:NE	1:A:460:ALA:HB1	2.34	0.43
1:A:688:TRP:HE1	1:A:722:VAL:HG13	1.84	0.43
2:B:63:U:N3	2:B:64:U:O4	2.51	0.43
1:A:578:SER:HB2	1:A:978:LEU:HD23	2.01	0.42
1:A:602:PHE:O	1:A:611:VAL:HG13	2.20	0.42
1:A:653:ARG:NH2	1:A:773:SER:O	2.53	0.42
1:A:79:ARG:HA	1:A:82:GLU:HB3	2.02	0.42
1:A:670:TRP:CH2	1:A:700:LYS:HG2	2.54	0.42
1:A:807:ASP:OD2	2:B:32:C:O2'	2.31	0.42
1:A:569:VAL:HG11	1:A:816:ILE:HD13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:C:O2'	2:B:93:A:OP1	2.17	0.42
1:A:79:ARG:NH2	1:A:83:ASN:OD1	2.52	0.42
1:A:581:VAL:HG21	1:A:616:ARG:CZ	2.51	0.41
1:A:79:ARG:HH21	1:A:189:PRO:HG2	1.86	0.41
1:A:26:HIS:O	1:A:30:ASN:ND2	2.37	0.41
1:A:341:LYS:HD3	1:A:344:GLU:HG3	2.03	0.41
1:A:969:GLY:HA2	1:A:1107:TYR:CD2	2.55	0.41
1:A:1080:ASP:OD2	1:A:1084:ILE:N	2.41	0.41
1:A:278:SER:HA	1:A:665:ARG:HH21	1.84	0.41
1:A:850:LEU:HB2	1:A:872:HIS:CE1	2.56	0.41
1:A:860:PRO:HB3	1:A:864:ASN:HB2	2.03	0.41
1:A:270:LEU:O	1:A:274:MSE:HG2	2.21	0.40
1:A:652:LEU:HD13	1:A:722:VAL:HG12	2.03	0.40
1:A:77:ARG:CZ	1:A:95:LEU:HD21	2.51	0.40
1:A:8:VAL:HG21	1:A:447:LEU:HD11	2.04	0.40
1:A:604:ILE:HG12	1:A:989:TRP:HB3	2.04	0.40
1:A:479:ALA:HA	1:A:503:ASN:O	2.22	0.40
1:A:8:VAL:HG11	1:A:441:ILE:HD13	2.04	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	936/1130 (83%)	877 (94%)	59 (6%)	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	829/947 (88%)	774 (93%)	55 (7%)	19	56

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	39	TRP
1	A	77	ARG
1	A	116	ASP
1	A	119	GLN
1	A	180	ARG
1	A	187	LEU
1	A	190	LEU
1	A	196	ASP
1	A	207	LEU
1	A	245	LEU
1	A	251	ARG
1	A	263	LEU
1	A	265	HIS
1	A	300	ASP
1	A	392	THR
1	A	400	ASN
1	A	402	HIS
1	A	410	GLU
1	A	426	VAL
1	A	427	GLU
1	A	503	ASN
1	A	540	ASP
1	A	541	LYS
1	A	548	GLU
1	A	555	LEU
1	A	588	ASP
1	A	602	PHE
1	A	607	ASN
1	A	616	ARG
1	A	618	GLN
1	A	661	GLU
1	A	666	ARG
1	A	670	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	716	TYR
1	A	742	ARG
1	A	752	VAL
1	A	758	ILE
1	A	855	PHE
1	A	857	ASN
1	A	876	PHE
1	A	893	MSE
1	A	932	LEU
1	A	977	ASP
1	A	985	GLN
1	A	988	LEU
1	A	994	ILE
1	A	1010	LEU
1	A	1029	VAL
1	A	1072	GLU
1	A	1073	LYS
1	A	1075	VAL
1	A	1077	LEU
1	A	1087	ARG
1	A	1099	MSE

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	76/112 (67%)	25 (32%)	3 (3%)

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	6	G
2	B	8	G
2	B	11	C
2	B	13	G
2	B	15	A
2	B	26	G
2	B	28	U
2	B	29	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	31	G
2	B	34	A
2	B	35	A
2	B	36	U
2	B	46	C
2	B	59	C
2	B	60	C
2	B	64	U
2	B	65	G
2	B	66	A
2	B	67	G
2	B	68	C
2	B	69	U
2	B	83	A
2	B	86	U
2	B	87	G
2	B	96	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	5	A
2	B	82	G
2	B	86	U

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 carbohydrates 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	942/1130 (83%)	0.70	110 (11%) 5 3	55, 109, 166, 216	0
2	B	78/112 (69%)	0.28	3 (3%) 41 32	70, 146, 263, 293	0
All	All	1020/1242 (82%)	0.67	113 (11%) 6 4	55, 111, 177, 293	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	333	PHE	8.9
1	A	328	ARG	7.6
1	A	334	GLY	6.2
1	A	599	PRO	6.0
1	A	933	ASN	5.8
1	A	11	ARG	5.2
1	A	297	ARG	5.0
1	A	394	PHE	5.0
1	A	347	TYR	4.8
1	A	272	GLN	4.7
1	A	482	GLN	4.5
1	A	483	CYS	4.5
1	A	95	LEU	4.5
1	A	342	LEU	4.3
2	B	82	G	4.3
1	A	301	LYS	4.2
1	A	76	LEU	4.2
1	A	327	ARG	4.0
1	A	276	GLU	3.9
1	A	204	TRP	3.9
1	A	914	ARG	3.8
1	A	737	VAL	3.7
1	A	776	PHE	3.7
1	A	270	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	0	G	3.6
1	A	402	HIS	3.6
1	A	213	VAL	3.5
1	A	335	SER	3.5
1	A	600	PHE	3.4
1	A	733	TRP	3.4
1	A	1108	LEU	3.4
1	A	659	GLY	3.4
1	A	194	TYR	3.3
1	A	1090	TRP	3.3
1	A	129	ALA	3.2
1	A	631	LEU	3.2
1	A	81	VAL	3.2
1	A	423	LEU	3.2
1	A	341	LYS	3.1
1	A	1025	TYR	3.1
2	B	15	A	3.0
1	A	1008	GLY	3.0
1	A	348	GLN	3.0
1	A	296	LEU	2.9
1	A	617	SER	2.9
1	A	29	VAL	2.9
1	A	426	VAL	2.9
1	A	934	LYS	2.8
1	A	618	GLN	2.8
1	A	12	LEU	2.8
1	A	8	VAL	2.8
1	A	550	PRO	2.8
1	A	547	ALA	2.8
1	A	89	ALA	2.8
1	A	401	LEU	2.7
1	A	847	LEU	2.7
1	A	75	ARG	2.7
1	A	295	ALA	2.7
1	A	380	PHE	2.7
1	A	655	LEU	2.6
1	A	542	LEU	2.6
1	A	1000	ARG	2.6
1	A	221	PHE	2.6
1	A	186	GLY	2.6
1	A	299	SER	2.6
1	A	388	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	126	SER	2.5
1	A	424	LEU	2.5
1	A	292	THR	2.5
1	A	628	SER	2.5
1	A	395	ASP	2.5
1	A	39	TRP	2.4
1	A	37	THR	2.4
1	A	389	PRO	2.4
1	A	834	LYS	2.4
1	A	855	PHE	2.4
1	A	734	ARG	2.4
1	A	390	ILE	2.4
1	A	106	LEU	2.3
1	A	479	ALA	2.3
1	A	546	LEU	2.3
1	A	193	VAL	2.3
1	A	697	GLN	2.3
1	A	582	PHE	2.3
1	A	77	ARG	2.3
1	A	10	LEU	2.3
1	A	819	GLU	2.2
1	A	639	GLN	2.2
1	A	187	LEU	2.2
1	A	692	PHE	2.2
1	A	699	LEU	2.2
1	A	821	LEU	2.2
1	A	1005	GLU	2.2
1	A	391	TRP	2.1
1	A	9	LYS	2.1
1	A	209	LYS	2.1
1	A	294	ARG	2.1
1	A	420	PHE	2.1
1	A	433	GLU	2.1
1	A	7	LYS	2.1
1	A	715	VAL	2.1
1	A	973	GLN	2.1
1	A	206	PRO	2.1
1	A	764	LEU	2.1
1	A	763	TYR	2.0
1	A	271	GLN	2.0
1	A	793	PHE	2.0
1	A	501	TYR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	300	ASP	2.0
1	A	765	GLU	2.0
1	A	291	VAL	2.0
1	A	45	GLN	2.0
1	A	812	LEU	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 carbohydrates 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.