



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 01:56 AM EST

PDB ID : 5U34
Title : Crystal structure of AacC2c1-sgRNA binary complex
Authors : Yang, H.; Gao, P.; Rajashankar, K.R.; Patel, D.J.
Deposited on : 2016-12-01
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

<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

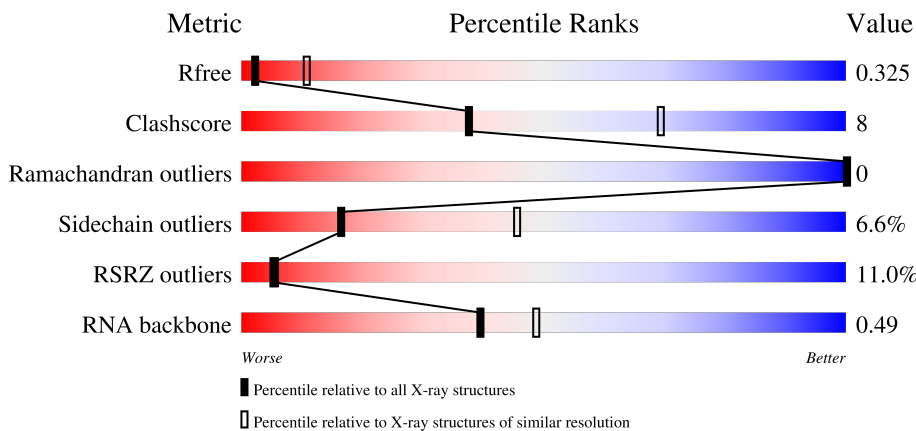
1 Overall quality at a glance

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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)
RNA backbone	3102	1072 (3.62-2.90)

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	1130	 10% 65% 18% • 15%
2	B	112	 3% 33% 35% • 30%

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
			Total	C	N	O	S	Se			
1	A	960	7882	4978	1458	1420	8	18	0	0	0

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

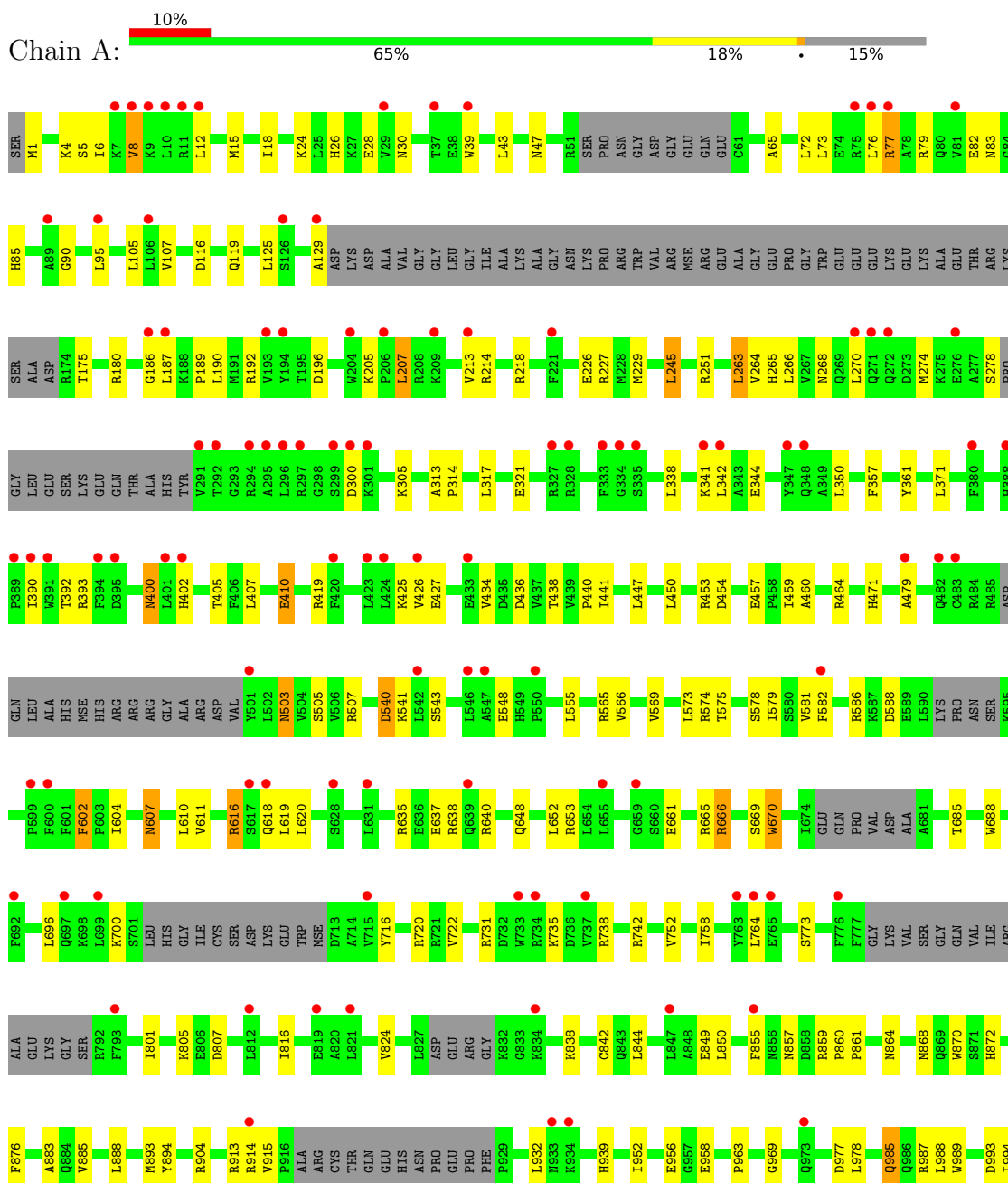
- Molecule 2 is a RNA chain called sgRNA.

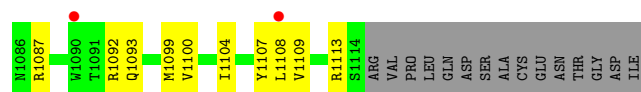
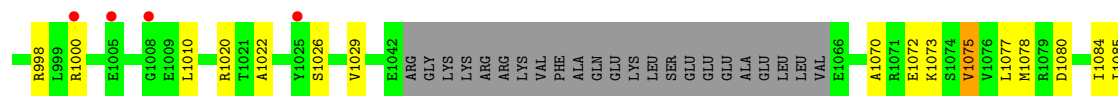
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	78	1680	749	315	538	78	0	0	0

3 Residue-property plots

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 C2c1





• Molecule 2: sgRNA



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)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.270 , 0.324 0.271 , 0.325	Depositor DCC
R_{free} test set	1302 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	112.4	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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

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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

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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:76:LEU:HD22	1:A:95:LEU:HG	1.92	0.52
1:A:648:GLN:OE1	1:A:685:THR:OG1	2.24	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: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:1078:MSE:HE3	1:A:1093:GLN:HG3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:H	1:A:207:LEU:HD23	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:HA	1:A:720:ARG:HD3	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:266:LEU:HB3	1:A:350:LEU:HD21	2.00	0.44
1:A:1000:ARG:NH2	1:A:1070:ALA:O	2.42	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:79:ARG:HA	1:A:82:GLU:HB3	2.02	0.42
1:A:653:ARG:NH2	1:A:773:SER:O	2.53	0.42
1:A:670:TRP:CH2	1:A:700:LYS:HG2	2.54	0.42
1:A:569:VAL:HG11	1:A:816:ILE:HD13	2.02	0.42
1:A:807:ASP:OD2	2:B:32:C:O2'	2.31	0.42

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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:79:ARG:HH21	1:A:189:PRO:HG2	1.86	0.41
1:A:581:VAL:HG21	1:A:616:ARG:CZ	2.51	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:278:SER:HA	1:A:665:ARG:HH21	1.84	0.41
1:A:1080:ASP:OD2	1:A:1084:ILE:N	2.41	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:77:ARG:CZ	1:A:95:LEU:HD21	2.51	0.40
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: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:8:VAL:HG11	1:A:441:ILE:HD13	2.04	0.40
1:A:479:ALA:HA	1:A:503:ASN:O	2.22	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	936/1130 (83%)	877 (94%)	59 (6%)	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	829/947 (88%)	774 (93%)	55 (7%)	16 45

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

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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

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	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

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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 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

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	109 (11%) 4 4	55, 109, 166, 216	0
2	B	78/112 (69%)	0.28	3 (3%) 40 37	70, 146, 263, 293	0
All	All	1020/1242 (82%)	0.67	112 (10%) 5 5	55, 111, 177, 293	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	333	PHE	8.8
1	A	328	ARG	7.7
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	4.4
1	A	342	LEU	4.4
1	A	301	LYS	4.3
2	B	82	G	4.3
1	A	76	LEU	4.2
1	A	327	ARG	4.0
1	A	276	GLU	4.0
1	A	204	TRP	3.8
1	A	914	ARG	3.8
1	A	737	VAL	3.7
1	A	776	PHE	3.7
1	A	270	LEU	3.6

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

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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	39	TRP	2.5
1	A	628	SER	2.5
1	A	395	ASP	2.4
1	A	834	LYS	2.4
1	A	37	THR	2.4
1	A	855	PHE	2.4
1	A	389	PRO	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	697	GLN	2.3
1	A	546	LEU	2.3
1	A	193	VAL	2.3
1	A	10	LEU	2.3
1	A	582	PHE	2.3
1	A	77	ARG	2.3
1	A	639	GLN	2.2
1	A	819	GLU	2.2
1	A	692	PHE	2.2
1	A	187	LEU	2.2
1	A	699	LEU	2.2
1	A	821	LEU	2.2
1	A	391	TRP	2.1
1	A	420	PHE	2.1
1	A	1005	GLU	2.1
1	A	9	LYS	2.1
1	A	209	LYS	2.1
1	A	294	ARG	2.1
1	A	973	GLN	2.1
1	A	715	VAL	2.1
1	A	433	GLU	2.1
1	A	7	LYS	2.1
1	A	763	TYR	2.1
1	A	764	LEU	2.1
1	A	271	GLN	2.0
1	A	300	ASP	2.0
1	A	291	VAL	2.0
1	A	501	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	206	PRO	2.0
1	A	793	PHE	2.0
1	A	812	LEU	2.0
1	A	765	GLU	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.