



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 04:37 pm BST

PDB ID : 5U33  
Title : Crystal structure of AacC2c1-sgRNA-extended non-target DNA ternary complex  
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Deposited on : 2016-12-01  
Resolution : 3.75 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](mailto: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.

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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	:	2.11
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)	:	2.11

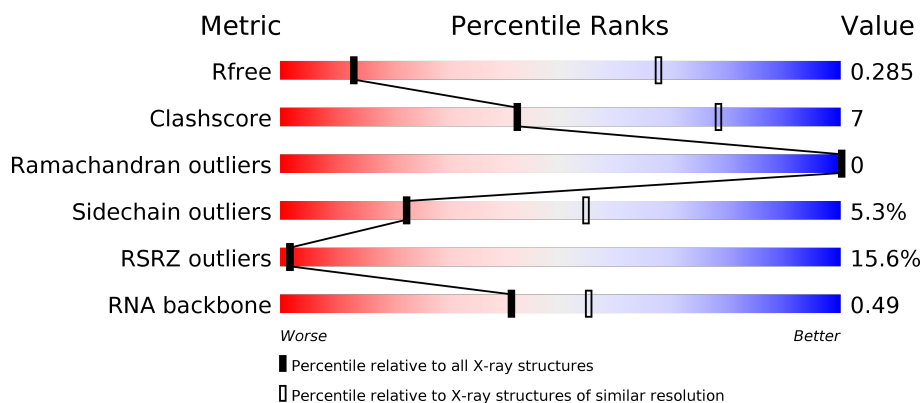
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.75 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	1039 (3.94-3.58)
Clashscore	141614	1051 (3.92-3.60)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RSRZ outliers	127900	1050 (3.96-3.56)
RNA backbone	3102	1035 (4.52-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>16%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
2	B	112	<div> <div>4%</div> <div> <div></div> <div>47%</div> <div>27%</div> <div>16%</div> <div>10%</div> </div> </div>
3	C	28	<div> <div></div> <div> <div></div> <div>71%</div> <div>29%</div> </div> </div>
4	D	28	<div> <div>4%</div> <div> <div></div> <div>39%</div> <div>11%</div> <div>50%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	1201	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11883 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	1085	Total	C	N	O	S	0	0	0
			8864	5569	1653	1611	31			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP T0D7A2
A	570	ALA	ASP	engineered mutation	UNP T0D7A2
A	848	ALA	GLU	engineered mutation	UNP T0D7A2
A	977	ALA	ASP	engineered mutation	UNP T0D7A2

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	101	Total	C	N	O	P	0	0	0
			2167	967	401	698	101			

- Molecule 3 is a DNA chain called Target DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	28	Total	C	N	O	P	0	0	0
			565	271	98	169	27			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	14	Total	C	N	O	P	0	0	0
			282	139	38	92	13			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

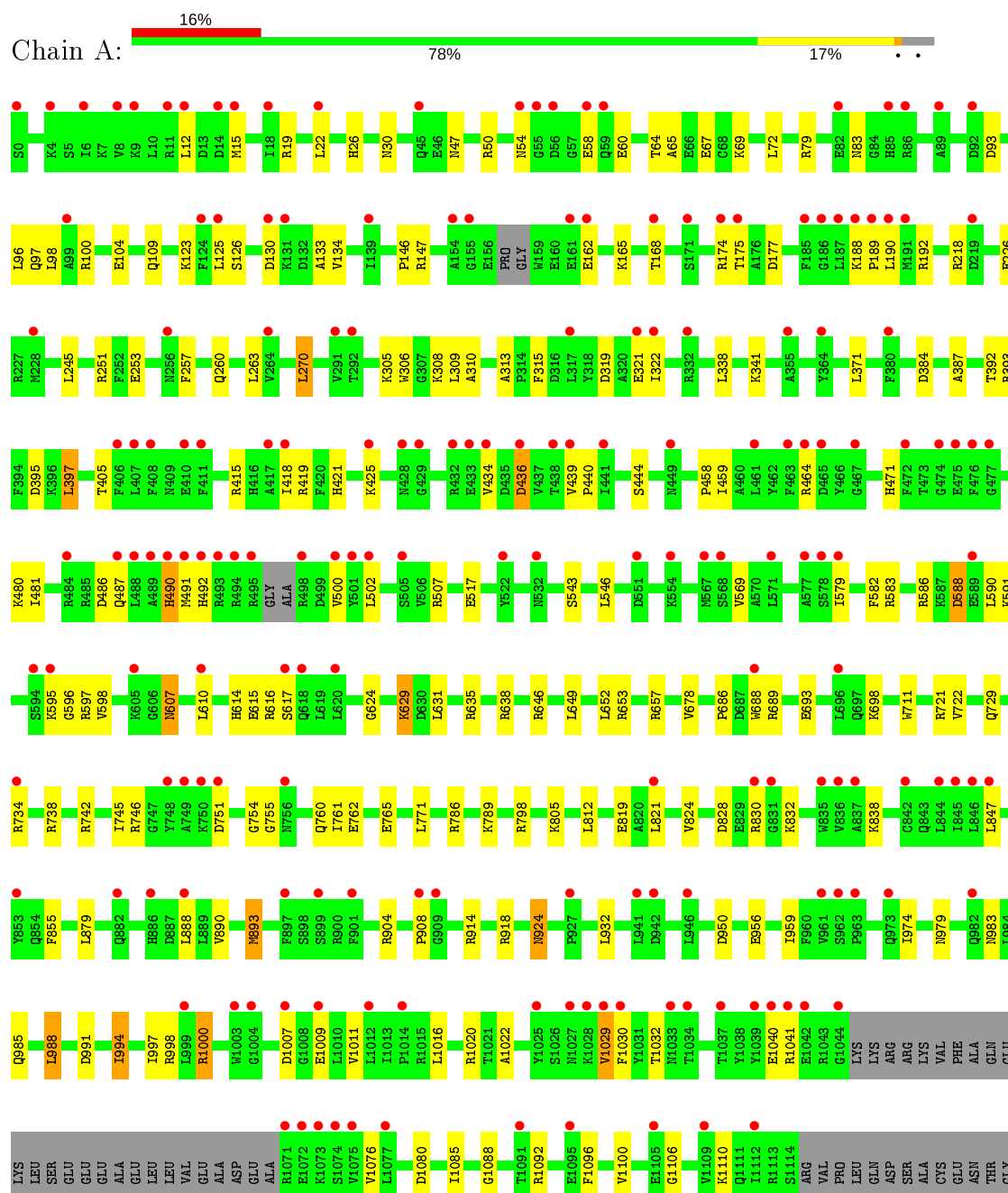


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



Category	Count
T1	100
G5	100
C8	100
T9	100
T102	100
T103	100
T104	100
DT	500

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.50Å 179.11Å 216.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 – 3.75 100.54 – 3.75	Depositor EDS
% Data completeness (in resolution range)	95.4 (47.49-3.75) 95.2 (100.54-3.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 3.78Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.245 , 0.286 0.247 , 0.285	Depositor DCC
$R_{free}$ test set	1126 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	134.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 101.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11883	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	148.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.26	1/9057 (0.0%)	0.40	0/12202
2	B	0.22	0/2424	0.82	0/3774
3	C	0.51	0/631	0.94	0/971
4	D	0.55	0/311	1.15	0/477
All	All	0.28	1/12423 (0.0%)	0.59	0/17424

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	GLU	CD-OE2	6.99	1.33	1.25

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	8864	0	8763	125	0
2	B	2167	0	1096	33	0
3	C	565	0	318	5	0
4	D	282	0	167	5	0
5	A	5	0	0	0	0
All	All	11883	0	10344	146	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 7.

All (146) 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:130:ASP:HB3	1:A:133:ALA:HB2	1.59	0.84
1:A:1085:ILE:HD13	1:A:1100:VAL:HG22	1.70	0.74
1:A:738:ARG:HB3	2:B:37:G:H5''	1.70	0.73
1:A:761:ILE:HD13	1:A:805:LYS:HG2	1.72	0.71
1:A:418:ILE:HD13	1:A:502:LEU:HD23	1.73	0.71
1:A:754:GLY:HA3	1:A:760:GLN:HG3	1.74	0.70
1:A:742:ARG:NH2	2:B:35:A:OP1	2.25	0.69
3:C:26:DA:H2''	3:C:27:DC:H5''	1.73	0.68
1:A:397:LEU:H	1:A:459:ILE:HD11	1.59	0.68
1:A:614:HIS:ND1	2:B:6:G:OP1	2.27	0.67
1:A:425:LYS:HE2	1:A:434:VAL:HG11	1.77	0.66
4:D:8:DC:H2''	4:D:9:DT:H5'	1.78	0.66
1:A:904:ARG:NH2	2:B:5:A:OP2	2.29	0.65
1:A:397:LEU:HD12	1:A:458:PRO:HG2	1.78	0.65
1:A:746:ARG:NH2	2:B:60:C:OP1	2.32	0.62
2:B:69:U:O2'	2:B:70:U:O5'	2.15	0.61
1:A:755:GLY:HA2	2:B:33:C:H4'	1.82	0.61
1:A:507:ARG:NH2	3:C:21:DG:OP1	2.34	0.60
1:A:125:LEU:HD23	1:A:218:ARG:HG2	1.84	0.60
1:A:218:ARG:NH1	4:D:5:DG:OP2	2.21	0.59
1:A:698:LYS:NZ	1:A:721:ARG:HH22	2.01	0.59
1:A:397:LEU:HG	1:A:405:THR:HG22	1.84	0.59
1:A:678:VAL:HG21	1:A:693:GLU:HG2	1.83	0.59
1:A:12:LEU:HD23	1:A:15:MET:HE3	1.83	0.59
1:A:54:ASN:HA	1:A:789:LYS:HE2	1.85	0.58
1:A:245:LEU:HB3	1:A:371:LEU:HD13	1.85	0.58
1:A:569:VAL:HG22	1:A:579:ILE:HG22	1.85	0.57
1:A:260:GLN:HB3	1:A:263:LEU:HD13	1.86	0.57
1:A:100:ARG:NE	1:A:104:GLU:OE2	2.38	0.57
1:A:569:VAL:HB	1:A:847:LEU:HD23	1.87	0.57
1:A:688:TRP:HB2	1:A:729:GLN:HE22	1.71	0.56
1:A:607:ASN:N	1:A:607:ASN:OD1	2.41	0.53
1:A:188:LYS:HB3	1:A:189:PRO:HD3	1.90	0.53
1:A:79:ARG:HH22	1:A:192:ARG:HG2	1.74	0.53
1:A:591:LYS:HB3	1:A:596:GLY:HA2	1.91	0.53
2:B:68:C:H42	2:B:85:G:H1	1.57	0.53
1:A:588:ASP:OD1	1:A:588:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:G:H2'	2:B:95:A:C8	2.45	0.52
1:A:69:LYS:HD3	1:A:96:LEU:HD13	1.92	0.52
1:A:22:LEU:HD22	1:A:481:ILE:HD13	1.92	0.51
1:A:847:LEU:HD11	1:A:879:LEU:HD12	1.91	0.51
1:A:123:LYS:HE2	1:A:175:THR:HG21	1.93	0.51
1:A:464:ARG:HG2	1:A:471:HIS:CE1	2.46	0.51
1:A:616:ARG:NH1	1:A:819:GLU:OE1	2.43	0.51
1:A:746:ARG:HH22	2:B:60:C:P	2.32	0.51
1:A:50:ARG:NH2	1:A:60:GLU:OE1	2.43	0.51
1:A:745:ILE:HD11	2:B:34:A:OP1	2.09	0.51
1:A:994:ILE:HD12	1:A:998:ARG:HB3	1.92	0.51
1:A:1000:ARG:HG2	1:A:1076:VAL:HG22	1.93	0.50
1:A:15:MET:HE1	1:A:440:PRO:HD2	1.92	0.50
1:A:991:ASP:O	1:A:1020:ARG:NH1	2.33	0.50
1:A:698:LYS:HZ2	1:A:721:ARG:HH22	1.59	0.50
1:A:745:ILE:HD12	1:A:745:ILE:H	1.77	0.50
1:A:147:ARG:NH2	4:D:9:DT:OP2	2.44	0.50
1:A:305:LYS:HA	1:A:308:LYS:HE2	1.94	0.50
1:A:543:SER:HB3	1:A:607:ASN:HD22	1.77	0.50
1:A:924:ASN:OD1	1:A:924:ASN:N	2.45	0.50
1:A:12:LEU:O	1:A:19:ARG:NH2	2.44	0.49
1:A:126:SER:OG	1:A:218:ARG:NH2	2.45	0.49
1:A:821:LEU:HG	1:A:888:LEU:HD11	1.93	0.49
1:A:79:ARG:NH2	1:A:192:ARG:HG2	2.27	0.49
2:B:106:A:H2'	2:B:107:A:C8	2.46	0.49
1:A:832:LYS:HZ3	2:B:85:G:H5''	1.78	0.49
3:C:9:DC:H2'	3:C:10:DC:C6	2.49	0.48
1:A:384:ASP:OD2	1:A:387:ALA:N	2.37	0.48
1:A:918:ARG:HG3	2:B:13:G:OP1	2.13	0.48
2:B:22:A:H4'	2:B:23:A:OP1	2.14	0.48
1:A:64:THR:HG23	1:A:67:GLU:H	1.78	0.48
1:A:15:MET:HE1	1:A:439:VAL:HA	1.96	0.48
2:B:87:G:O2'	2:B:88:G:H5''	2.14	0.48
1:A:653:ARG:O	1:A:657:ARG:HG3	2.14	0.47
1:A:270:LEU:HD21	1:A:341:LYS:HG2	1.97	0.47
2:B:20:U:H5	2:B:86:U:H2'	1.79	0.47
1:A:819:GLU:OE2	2:B:8:G:N1	2.37	0.47
2:B:21:C:H2'	2:B:22:A:H5'	1.95	0.47
1:A:614:HIS:NE2	1:A:617:SER:OG	2.40	0.47
1:A:635:ARG:HA	1:A:638:ARG:HD2	1.96	0.46
1:A:415:ARG:NH2	2:B:27:G:OP1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:C:N4	2:B:69:U:O4	2.48	0.46
1:A:47:ASN:OD1	1:A:65:ALA:N	2.48	0.46
1:A:93:ASP:OD1	1:A:97:GLN:NE2	2.49	0.46
1:A:1009:GLU:HG3	1:A:1011:VAL:HG13	1.97	0.45
1:A:762:GLU:HA	1:A:765:GLU:HB2	1.98	0.45
1:A:824:VAL:HB	1:A:838:LYS:HD3	1.99	0.45
1:A:405:THR:OG1	1:A:419:ARG:HB3	2.16	0.45
1:A:319:ASP:HA	1:A:322:ILE:HD12	1.98	0.45
1:A:147:ARG:HH21	4:D:9:DT:H2'	1.82	0.45
1:A:109:GLN:OE1	1:A:109:GLN:N	2.47	0.44
1:A:405:THR:HG23	1:A:421:HIS:NE2	2.32	0.44
1:A:985:GLN:HE21	1:A:985:GLN:HB2	1.65	0.44
1:A:624:GLY:HA3	1:A:754:GLY:O	2.18	0.44
1:A:226:GLU:OE2	1:A:393:ARG:NH2	2.48	0.44
1:A:646:ARG:NH2	3:C:1:DG:O5'	2.50	0.44
1:A:828:ASP:C	1:A:830:ARG:H	2.21	0.44
1:A:486:ASP:OD1	1:A:487:GLN:N	2.51	0.44
1:A:26:HIS:CE1	1:A:30:ASN:HD21	2.36	0.44
1:A:444:SER:HA	2:B:29:G:C8	2.53	0.44
1:A:490:HIS:HB3	1:A:492:HIS:CD2	2.53	0.43
1:A:734:ARG:HD2	1:A:771:LEU:HD21	1.99	0.43
1:A:1096:PHE:O	1:A:1100:VAL:HG23	2.18	0.43
1:A:689:ARG:HE	1:A:689:ARG:HB3	1.59	0.43
1:A:146:PRO:HG3	4:D:8:DC:OP1	2.18	0.43
1:A:893:MET:HE3	1:A:988:LEU:HA	2.01	0.43
1:A:1029:VAL:HG12	1:A:1041:ARG:HB2	1.99	0.43
1:A:974:ILE:HG23	1:A:979:ASN:HB2	1.99	0.43
1:A:653:ARG:NH2	2:B:105:C:H5''	2.33	0.43
1:A:1029:VAL:O	1:A:1041:ARG:N	2.47	0.43
1:A:174:ARG:NH1	1:A:177:ASP:OD1	2.48	0.43
1:A:914:ARG:HE	1:A:959:ILE:HD13	1.83	0.43
2:B:5:A:O2'	2:B:6:G:O5'	2.33	0.43
1:A:22:LEU:HD13	1:A:500:VAL:HG11	2.00	0.42
1:A:751:ASP:N	1:A:751:ASP:OD1	2.52	0.42
1:A:147:ARG:NH1	1:A:162:GLU:OE1	2.52	0.42
1:A:83:ASN:ND2	1:A:189:PRO:HD2	2.33	0.42
1:A:1016:LEU:HG	1:A:1022:ALA:HA	2.00	0.42
1:A:631:LEU:HD11	1:A:751:ASP:HB3	2.02	0.42
1:A:1080:ASP:HB3	1:A:1088:GLY:HA2	2.01	0.42
1:A:306:TRP:HZ2	1:A:322:ILE:HD11	1.84	0.42
1:A:543:SER:HB3	1:A:607:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:LEU:HD23	1:A:879:LEU:HA	1.89	0.42
2:B:21:C:OP1	2:B:21:C:H6	2.03	0.42
2:B:33:C:H5''	2:B:34:A:C5'	2.50	0.42
1:A:1106:GLY:O	1:A:1110:LYS:HD2	2.20	0.42
1:A:15:MET:CE	1:A:440:PRO:HD2	2.50	0.42
2:B:21:C:P	2:B:21:C:O4'	2.78	0.41
1:A:165:LYS:HA	1:A:168:THR:HG22	2.01	0.41
1:A:688:TRP:HB2	1:A:729:GLN:NE2	2.34	0.41
1:A:310:ALA:HB3	1:A:313:ALA:HB2	2.03	0.41
1:A:832:LYS:NZ	2:B:85:G:H5''	2.35	0.41
1:A:305:LYS:HB3	1:A:321:GLU:CG	2.50	0.41
3:C:15:DG:H2''	3:C:16:DT:H5'	2.02	0.41
1:A:419:ARG:HD3	1:A:436:ASP:OD1	2.20	0.41
1:A:546:LEU:HA	1:A:546:LEU:HD23	1.94	0.41
1:A:686:PRO:HA	1:A:689:ARG:HH21	1.85	0.41
2:B:56:A:H2'	2:B:57:A:O4'	2.21	0.41
1:A:629:LYS:CD	1:A:629:LYS:H	2.33	0.41
1:A:1030:PHE:CE1	1:A:1040:GLU:HG2	2.55	0.41
2:B:67:G:C2	2:B:68:C:C2	3.08	0.41
1:A:586:ARG:HA	1:A:610:LEU:HD23	2.03	0.41
2:B:30:U:H2'	2:B:31:G:O4'	2.21	0.41
1:A:908:PRO:HG3	1:A:1096:PHE:CZ	2.57	0.40
2:B:72:U:H2'	2:B:73:C:H6	1.86	0.40
1:A:397:LEU:HD23	1:A:397:LEU:HA	1.73	0.40
1:A:657:ARG:NH1	2:B:108:A:OP2	2.55	0.40
1:A:582:PHE:CE2	1:A:614:HIS:HD2	2.39	0.40
1:A:583:ARG:NE	1:A:615:GLU:OE2	2.41	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	1077/1130 (95%)	1021 (95%)	56 (5%)	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	930/966 (96%)	881 (95%)	49 (5%)	22	54

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	LEU
1	A	98	LEU
1	A	134	VAL
1	A	190	LEU
1	A	251	ARG
1	A	253	GLU
1	A	257	PHE
1	A	270	LEU
1	A	309	LEU
1	A	315	PHE
1	A	338	LEU
1	A	392	THR
1	A	395	ASP
1	A	397	LEU
1	A	436	ASP
1	A	480	LYS
1	A	490	HIS
1	A	491	MET
1	A	517	GLU
1	A	588	ASP
1	A	590	LEU
1	A	595	LYS
1	A	597	ARG

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Mol	Chain	Res	Type
1	A	598	VAL
1	A	607	ASN
1	A	629	LYS
1	A	649	LEU
1	A	652	LEU
1	A	711	TRP
1	A	722	VAL
1	A	786	ARG
1	A	798	ARG
1	A	812	LEU
1	A	855	PHE
1	A	890	VAL
1	A	893	MET
1	A	924	ASN
1	A	932	LEU
1	A	950	ASP
1	A	956	GLU
1	A	983	ASN
1	A	988	LEU
1	A	994	ILE
1	A	997	ILE
1	A	1000	ARG
1	A	1007	ASP
1	A	1029	VAL
1	A	1032	THR
1	A	1092	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	99/112 (88%)	28 (28%)	5 (5%)

All (28) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	5	A
2	B	6	G
2	B	12	A
2	B	13	G
2	B	16	U
2	B	21	C
2	B	22	A
2	B	23	A
2	B	29	G
2	B	31	G
2	B	33	C
2	B	34	A
2	B	36	U
2	B	46	C
2	B	57	A
2	B	58	G
2	B	60	C
2	B	66	A
2	B	67	G
2	B	68	C
2	B	69	U
2	B	70	U
2	B	83	A
2	B	87	G
2	B	93	A
2	B	101	A
2	B	102	G
2	B	111	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	5	A
2	B	22	A
2	B	32	C
2	B	82	G
2	B	86	U

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	SO4	A	1201	-	4,4,4	0.14	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	10:DT	O3'	101:DT	P	48.98

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1085/1130 (96%)	0.96	185 (17%) <b>1</b> <b>1</b>	87, 138, 195, 230	0
2	B	101/112 (90%)	0.28	5 (4%) 28 26	100, 156, 257, 271	0
3	C	28/28 (100%)	-0.37	0 <b>100</b> <b>100</b>	98, 130, 149, 161	0
4	D	14/28 (50%)	0.25	1 (7%) 16 12	122, 133, 191, 216	0
All	All	1228/1298 (94%)	0.86	191 (15%) <b>2</b> <b>2</b>	87, 139, 202, 271	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	HIS	11.9
1	A	495	ARG	8.7
1	A	494	ARG	7.7
1	A	155	GLY	7.4
1	A	493	ARG	7.4
1	A	490	HIS	7.1
1	A	1044	GLY	6.5
1	A	1071	ARG	5.7
1	A	1041	ARG	5.0
1	A	491	MET	4.8
1	A	1072	GLU	4.7
1	A	595	LYS	4.6
1	A	578	SER	4.6
1	A	417	ALA	4.5
1	A	475	GLU	4.5
1	A	406	PHE	4.5
1	A	256	ASN	4.3
1	A	909	GLY	4.2
1	A	488	LEU	4.0
1	A	846	LEU	4.0
1	A	749	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	438	THR	4.0
1	A	489	ALA	4.0
1	A	467	GLY	3.9
1	A	11	ARG	3.8
1	A	92	ASP	3.7
1	A	407	LEU	3.7
1	A	1030	PHE	3.6
1	A	15	MET	3.6
1	A	425	LYS	3.5
1	A	963	PRO	3.5
1	A	1074	SER	3.5
1	A	171	SER	3.5
1	A	58	GLU	3.4
1	A	696	LEU	3.4
1	A	973	GLN	3.4
1	A	831	GLY	3.3
1	A	441	ILE	3.3
1	A	942	ASP	3.3
1	A	463	PHE	3.3
1	A	436	ASP	3.3
1	A	1029	VAL	3.2
1	A	18	ILE	3.2
1	A	594	SER	3.2
1	A	1075	VAL	3.2
1	A	551	ASP	3.1
1	A	9	LYS	3.1
1	A	82	GLU	3.1
1	A	186	GLY	3.1
1	A	1003	TRP	3.1
1	A	291	VAL	3.0
1	A	464	ARG	3.0
1	A	579	ILE	3.0
1	A	317	LEU	3.0
1	A	59	GLN	3.0
1	A	131	LYS	3.0
1	A	439	VAL	3.0
1	A	487	GLN	3.0
1	A	14	ASP	3.0
1	A	1105	GLU	3.0
1	A	620	LEU	3.0
2	B	16	U	3.0
1	A	45	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	162	GLU	2.9
1	A	1033	ASN	2.9
1	A	139	ILE	2.9
1	A	1040	GLU	2.9
1	A	125	LEU	2.9
1	A	484	ARG	2.9
1	A	190	LEU	2.9
1	A	941	LEU	2.9
1	A	321	GLU	2.8
1	A	577	ALA	2.8
1	A	1009	GLU	2.8
1	A	1073	LYS	2.8
1	A	835	TRP	2.7
1	A	899	SER	2.7
1	A	187	LEU	2.7
1	A	610	LEU	2.7
1	A	962	SER	2.7
1	A	411	PHE	2.7
1	A	1028	LYS	2.7
1	A	292	THR	2.7
1	A	1037	THR	2.7
1	A	189	PRO	2.7
1	A	54	ASN	2.7
1	A	505	SER	2.7
1	A	897	PHE	2.7
1	A	465	ASP	2.7
4	D	102	DT	2.7
1	A	0	SER	2.7
1	A	418	ILE	2.7
1	A	6	ILE	2.7
1	A	175	THR	2.7
1	A	501	TYR	2.6
1	A	476	PHE	2.6
1	A	1004	GLY	2.6
1	A	1007	ASP	2.6
1	A	1042	GLU	2.6
1	A	264	VAL	2.6
1	A	191	MET	2.6
1	A	946	LEU	2.6
1	A	12	LEU	2.6
1	A	908	PRO	2.6
1	A	124	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	845	ILE	2.6
1	A	901	PHE	2.5
1	A	605	LYS	2.5
1	A	750	LYS	2.5
1	A	1112	ILE	2.5
1	A	174	ARG	2.5
1	A	89	ALA	2.5
1	A	844	LEU	2.5
1	A	837	ALA	2.5
1	A	433	GLU	2.5
1	A	1077	LEU	2.5
1	A	472	PHE	2.5
1	A	888	LEU	2.5
1	A	428	ASN	2.4
1	A	756	ASN	2.4
1	A	847	LEU	2.4
1	A	1025	TYR	2.4
1	A	408	PHE	2.4
1	A	85	HIS	2.4
1	A	1109	VAL	2.4
1	A	86	ARG	2.4
1	A	56	ASP	2.4
1	A	554	LYS	2.4
1	A	130	ASP	2.4
1	A	500	VAL	2.4
1	A	185	PHE	2.4
1	A	882	GLN	2.3
1	A	449	ASN	2.3
1	A	618	GLN	2.3
1	A	1027	ASN	2.3
1	A	99	ALA	2.3
1	A	567	MET	2.3
1	A	1014	PRO	2.3
1	A	1091	THR	2.3
1	A	999	LEU	2.3
1	A	1039	TYR	2.3
1	A	477	GLY	2.3
1	A	228	MET	2.3
1	A	161	GLU	2.3
1	A	830	ARG	2.3
1	A	571	LEU	2.3
1	A	821	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	532	ASN	2.2
1	A	332	ARG	2.2
1	A	4	LYS	2.2
1	A	589	GLU	2.2
1	A	617	SER	2.2
1	A	22	LEU	2.2
1	A	688	TRP	2.2
1	A	751	ASP	2.2
1	A	364	TYR	2.2
1	A	748	TYR	2.2
1	A	568	SER	2.2
1	A	522	TYR	2.2
1	A	961	VAL	2.2
1	A	55	GLY	2.2
1	A	886	HIS	2.2
1	A	853	TYR	2.1
1	A	1095	GLU	2.1
1	A	154	ALA	2.1
1	A	168	THR	2.1
1	A	1012	LEU	2.1
1	A	842	CYS	2.1
2	B	0	G	2.1
1	A	461	LEU	2.1
1	A	410	GLU	2.1
1	A	836	VAL	2.1
1	A	982	GLN	2.1
2	B	73	C	2.1
1	A	502	LEU	2.1
1	A	734	ARG	2.1
1	A	434	VAL	2.1
1	A	355	ALA	2.1
1	A	498	ARG	2.0
1	A	1034	THR	2.0
1	A	380	PHE	2.0
2	B	20	U	2.0
2	B	44	U	2.0
1	A	8	VAL	2.0
1	A	429	GLY	2.0
1	A	927	PRO	2.0
1	A	219	ASP	2.0
1	A	322	ILE	2.0
1	A	188	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	432	ARG	2.0
1	A	474	GLY	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	1201	5/5	0.76	0.44	143,143,149,152	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.