



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:58 AM UTC

PDB ID : 5U33 / pdb_00005u33
Title : Crystal structure of AacC2c1-sgRNA-extended non-target DNA ternary complex
Authors : Yang, H.; Gao, P.; Rajashankar, K.R.; Patel, D.J.
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

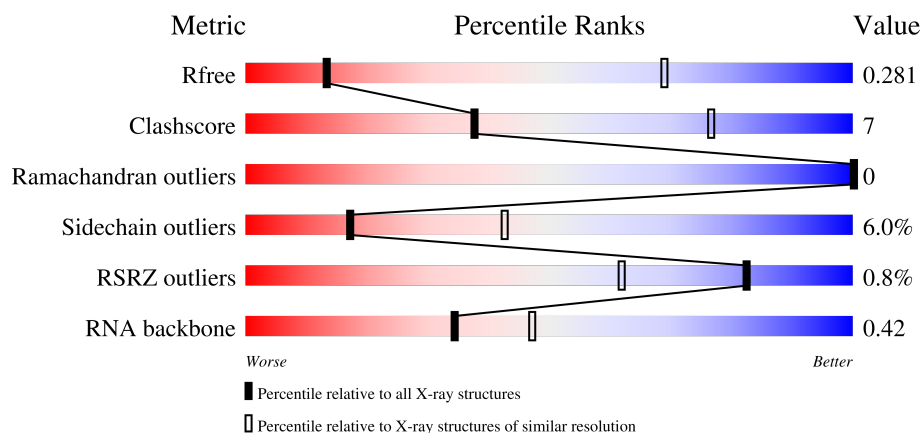
1 Overall quality at a glance

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}	180053	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)
RNA backbone	3983	1001 (4.40-3.10)

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	77% 17% . .
2	B	112	47% 27% 16% 10%
3	C	28	71% 29%
4	D	28	39% 11% 50%

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 (CCD ID: SO4) (formula: O₄S).

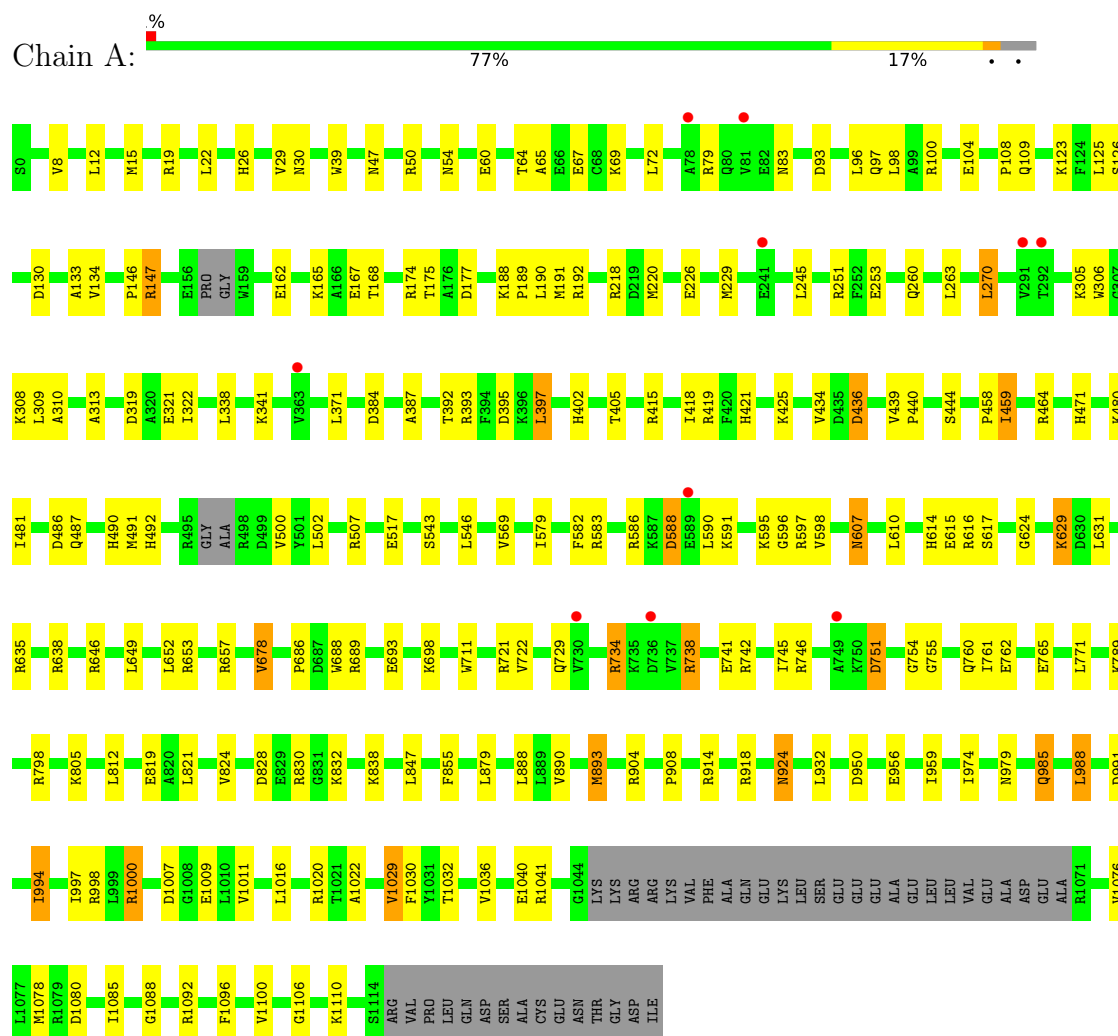


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

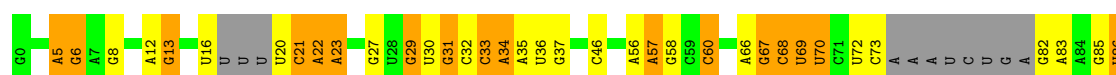
3 Residue-property plots

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

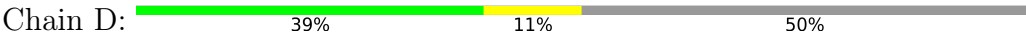




● Molecule 3: Target DNA strand



● Molecule 4: Non-target DNA strand



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	113.50Å 179.11Å 216.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.49 – 3.75 47.49 – 3.75	Depositor EDS
% Data completeness (in resolution range)	95.4 (47.49-3.75) 95.1 (47.49-3.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.78Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.245 , 0.286 0.247 , 0.281	Depositor DCC
R_{free} test set	1126 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	134.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 103.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11883	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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](#)

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	0.13	0/9057	0.31	0/12202
2	B	0.13	0/2424	0.36	0/3774
3	C	0.19	0/631	0.37	0/971
4	D	0.22	0/311	0.47	0/477
All	All	0.14	0/12423	0.33	0/17424

There are no bond length outliers.

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	128	0
2	B	2167	0	1096	31	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	148	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 (148) 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
2:B:69:U:O2'	2:B:70:U:O5'	2.15	0.63
1:A:746:ARG:NH2	2:B:60:C:OP1	2.32	0.62
1:A:12:LEU:HD23	1:A:15:MET:HE3	1.81	0.62
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: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:698:LYS:HZ2	1:A:721:ARG:HH22	1.52	0.56
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:991:ASP:O	1:A:1020:ARG:NH1	2.33	0.50
1:A:1000:ARG:HG2	1:A:1076:VAL:HG22	1.93	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:N	1:A:924:ASN:OD1	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:828:ASP:C	1:A:830:ARG:H	2.21	0.49
1:A:29:VAL:HA	1:A:220:MET:HE2	1.95	0.48
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
1:A:998:ARG:HD2	1:A:1078:MET:HE1	1.96	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
2:B:87:G:O2'	2:B:88:G:H5''	2.14	0.48
1:A:15:MET:HE1	1:A:439:VAL:HA	1.96	0.47
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:415:ARG:NH2	2:B:27:G:OP1	2.48	0.46
1:A:635:ARG:HA	1:A:638:ARG:HD2	1.96	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:15:MET:HE1	1:A:440:PRO:HD2	1.98	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: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:39:TRP:HB3	1:A:191:MET:HE2	2.00	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:653:ARG:NH2	2:B:105:C:H5''	2.33	0.43
1:A:974:ILE:HG23	1:A:979:ASN:HB2	1.99	0.43
1:A:1029:VAL:HG12	1:A:1041:ARG:HB2	1.99	0.43
1:A:174:ARG:NH1	1:A:177:ASP:OD1	2.48	0.43
1:A:1029:VAL:O	1:A:1041:ARG:N	2.47	0.43
1:A:914:ARG:HE	1:A:959:ILE:HD13	1.83	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:83:ASN:ND2	1:A:189:PRO:HD2	2.33	0.42
1:A:147:ARG:NH1	1:A:162:GLU:OE1	2.52	0.42
1:A:631:LEU:HD11	1:A:751:ASP:HB3	2.02	0.42
1:A:1016:LEU:HG	1:A:1022:ALA:HA	2.00	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
1:A:879:LEU:HD23	1:A:879:LEU:HA	1.89	0.42
1:A:1080:ASP:HB3	1:A:1088:GLY:HA2	2.01	0.42
2:B:21:C:OP1	2:B:21:C:H6	2.03	0.42
1:A:893:MET:HE3	1:A:988:LEU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:C:H5''	2:B:34:A:C5'	2.50	0.42
1:A:15:MET:CE	1:A:440:PRO:HD2	2.50	0.42
1:A:1106:GLY:O	1:A:1110:LYS:HD2	2.20	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:HD23	1:A:546:LEU:HA	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
1:A:108:PRO:HD2	1:A:229:MET:HE2	2.03	0.40
2:B:72:U:H2'	2:B:73:C:H6	1.86	0.40
1:A:397:LEU:HA	1:A:397:LEU:HD23	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%)	874 (94%)	56 (6%)	17	43

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	72	LEU
1	A	98	LEU
1	A	134	VAL
1	A	147	ARG
1	A	167	GLU
1	A	190	LEU
1	A	251	ARG
1	A	253	GLU
1	A	270	LEU
1	A	309	LEU
1	A	338	LEU
1	A	392	THR
1	A	395	ASP
1	A	397	LEU
1	A	402	HIS
1	A	436	ASP
1	A	459	ILE
1	A	480	LYS
1	A	491	MET
1	A	517	GLU
1	A	588	ASP
1	A	590	LEU

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Mol	Chain	Res	Type
1	A	595	LYS
1	A	597	ARG
1	A	598	VAL
1	A	607	ASN
1	A	629	LYS
1	A	649	LEU
1	A	652	LEU
1	A	678	VAL
1	A	711	TRP
1	A	722	VAL
1	A	734	ARG
1	A	738	ARG
1	A	741	GLU
1	A	751	ASP
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	985	GLN
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	1036	VAL
1	A	1092	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	639	GLN
1	A	648	GLN
1	A	682	ASN
1	A	729	GLN
1	A	803	HIS

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Mol	Chain	Res	Type
1	A	939	HIS
1	A	1033	ASN

5.3.3 RNA ⓘ

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 [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	0.23	0	6,6,6	0.08	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 [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, 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	1085/1130 (96%)	-0.06	10 (0%) 81 59	87, 138, 195, 230	0
2	B	101/112 (90%)	-0.20	0 100 100	100, 156, 257, 271	0
3	C	28/28 (100%)	-0.21	0 100 100	98, 130, 149, 161	0
4	D	14/28 (50%)	-0.06	0 100 100	122, 133, 191, 216	0
All	All	1228/1298 (94%)	-0.07	10 (0%) 82 62	87, 139, 202, 271	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	VAL	3.6
1	A	749	ALA	2.8
1	A	78	ALA	2.8
1	A	291	VAL	2.3
1	A	241	GLU	2.3
1	A	736	ASP	2.2
1	A	292	THR	2.1
1	A	589	GLU	2.1
1	A	730	VAL	2.1
1	A	81	VAL	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 oligosaccharides in this entry.

6.4 Ligands

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, 95th 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	0.88	0.11	143,143,149,152	0

6.5 Other polymers

There are no such residues in this entry.