



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:40 PM UTC

PDB ID : 5FW3 / pdb_00005fw3
Title : Crystal structure of SpCas9 variant VRER bound to sgRNA and TGCG PAM target DNA
Authors : Anders, C.; Bargsten, K.; Jinek, M.
Deposited on : 2016-02-11
Resolution : 2.70 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
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

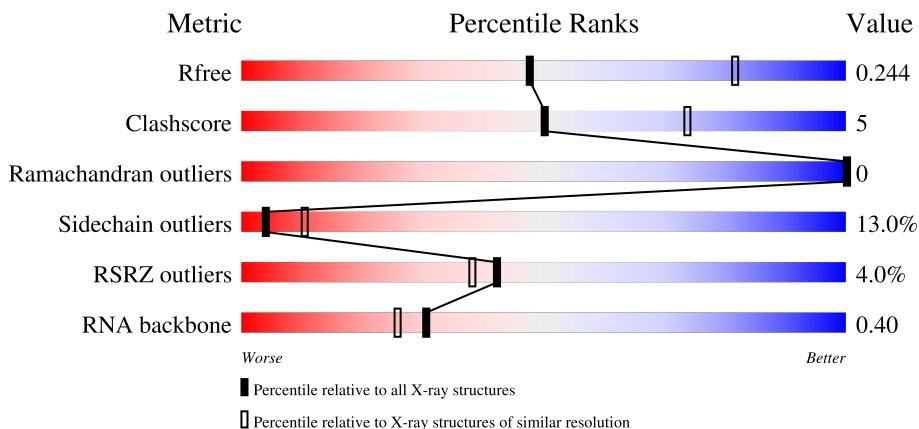
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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	83	2% 45% 36% 17% •
2	B	1372	4% 76% 17% • •
3	C	28	61% 39%
4	D	12	8% 50% 42% 8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25841 atoms, of which 12327 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 RNA chain called SGRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	81	Total	C	H	N	O	P	0	0	0
			2601	778	869	318	555	81			

- Molecule 2 is a protein called CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	1322	Total	C	H	N	O	S	0	0	0
			21835	6900	11011	1880	2022	22			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP Q99ZW2
B	-2	ALA	-	expression tag	UNP Q99ZW2
B	-1	ALA	-	expression tag	UNP Q99ZW2
B	0	SER	-	expression tag	UNP Q99ZW2
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
B	1135	VAL	ASP	engineered mutation	UNP Q99ZW2
B	1218	ARG	GLY	engineered mutation	UNP Q99ZW2
B	1335	GLU	ARG	engineered mutation	UNP Q99ZW2
B	1337	ARG	THR	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called TARGET DNA STRAND.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	28	Total	C	H	N	O	P	0	0	0
			888	275	321	97	168	27			

- Molecule 4 is a DNA chain called NON-TARGET DNA STRAND.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	11	Total	C	H	N	O	P	0	0	0
			352	109	126	44	63	10			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	K	0	0
			2	2		
6	B	9	Total	K	0	0
			9	9		

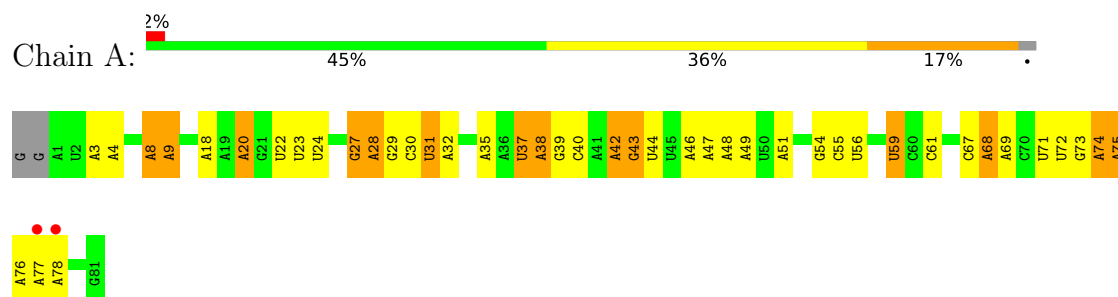
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	54	Total	O	0	0
			54	54		
7	B	93	Total	O	0	0
			93	93		
7	C	5	Total	O	0	0
			5	5		

3 Residue-property plots [i](#)

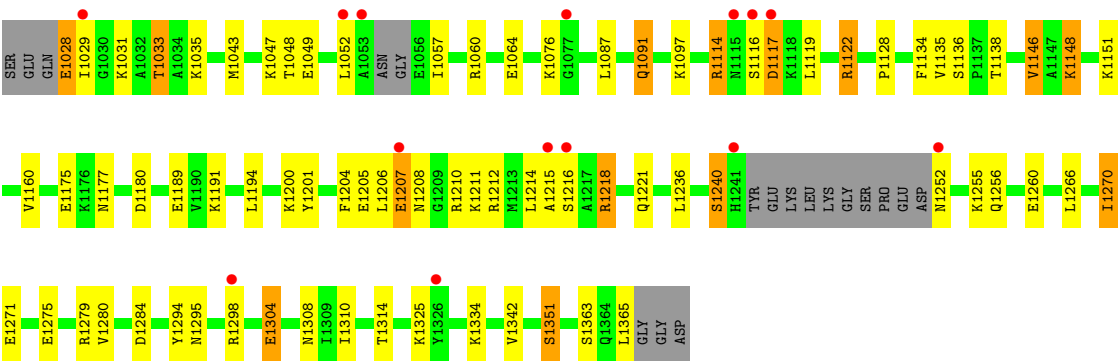
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SGRNA

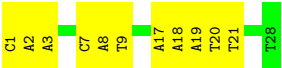


• Molecule 2: CRISPR-ASSOCIATED ENDONUCLEASE CAS9/CSN1





● Molecule 3: TARGET DNA STRAND



● Molecule 4: NON-TARGET DNA STRAND



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.52Å 67.80Å 187.70Å 90.00° 111.15° 90.00°	Depositor
Resolution (Å)	47.98 – 2.70 47.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.98-2.70) 100.0 (47.98-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.214 , 0.242 0.216 , 0.244	Depositor DCC
R_{free} test set	2887 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25841	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: MG, K

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	0.19	0/1942	0.43	0/3023
2	B	0.16	0/11012	0.36	0/14793
3	C	0.25	0/634	0.52	0/976
4	D	0.36	0/254	0.63	0/391
All	All	0.17	0/13842	0.39	0/19183

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	1732	869	869	27	0
2	B	10824	11011	11010	104	1
3	C	567	321	321	9	0
4	D	226	126	126	8	0
5	A	2	0	0	0	0
6	A	2	0	0	0	0
6	B	9	0	0	0	0
7	A	54	0	0	3	0
7	B	93	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	5	0	0	0	0
All	All	13514	12327	12326	137	1

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 5.

All (137) 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)
2:B:557:ARG:NH2	2:B:596:ASP:OD1	2.03	0.91
2:B:1207:GLU:OE2	2:B:1210:ARG:NH1	2.07	0.88
2:B:1236:LEU:O	2:B:1240:SER:OG	1.94	0.86
2:B:1114:ARG:NH1	4:D:9:DA:OP1	2.11	0.83
1:A:20:A:OP2	2:B:403:ARG:NH1	2.12	0.82
1:A:77:A:OP1	2:B:721:HIS:NE2	2.13	0.82
2:B:106:LEU:O	2:B:111:LYS:NZ	2.16	0.78
2:B:1212:ARG:NH2	2:B:1280:VAL:O	2.18	0.77
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.16	0.77
2:B:584:GLU:OE1	7:B:2043:HOH:O	2.03	0.75
2:B:1028:GLU:N	7:B:2070:HOH:O	2.22	0.71
2:B:1334:LYS:NZ	3:C:3:DA:OP2	2.24	0.70
2:B:809:GLU:OE1	7:B:2056:HOH:O	2.12	0.67
1:A:9:A:OP1	7:A:2004:HOH:O	2.12	0.67
7:A:2016:HOH:O	2:B:125:GLU:OE1	2.12	0.67
7:A:2044:HOH:O	2:B:69:ARG:NH2	2.27	0.67
2:B:633:GLU:OE1	2:B:652:LYS:NZ	2.27	0.66
2:B:388:GLU:OE1	7:B:2023:HOH:O	2.13	0.66
2:B:1205:GLU:OE2	7:B:2085:HOH:O	2.13	0.66
2:B:1047:LYS:O	2:B:1076:LYS:NZ	2.29	0.65
2:B:1177:ASN:ND2	2:B:1180:ASP:OD2	2.30	0.64
3:C:20:DT:H2'	3:C:21:DT:H71	1.80	0.63
2:B:139:ARG:NH1	2:B:418:GLU:OE1	2.34	0.61
2:B:954:LYS:NZ	2:B:1005:GLU:OE2	2.33	0.61
1:A:67:C:OP2	2:B:1097:LYS:NZ	2.34	0.61
1:A:73:G:H3'	1:A:74:A:H5''	1.81	0.61
2:B:204:SER:O	2:B:204:SER:OG	2.19	0.60
2:B:118:ILE:N	2:B:125:GLU:OE2	2.34	0.60
2:B:78:ARG:NH1	2:B:162:ILE:O	2.36	0.59
1:A:59:U:OP1	2:B:467:ARG:NH2	2.36	0.59
2:B:614:ASP:OD1	2:B:664:ARG:NH2	2.37	0.58
2:B:1304:GLU:O	2:B:1308:ASN:ND2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1218:ARG:NH2	4:D:8:DG:OP2	2.36	0.57
1:A:42:A:O2'	1:A:43:G:OP1	2.21	0.57
2:B:923:GLU:OE2	2:B:925:ARG:NH1	2.38	0.56
1:A:73:G:C3'	1:A:74:A:H5''	2.36	0.56
2:B:1295:ASN:OD1	2:B:1298:ARG:NH1	2.39	0.55
2:B:165:ARG:NH2	2:B:446:PHE:O	2.39	0.55
3:C:1:DC:H2'	3:C:2:DA:C8	2.42	0.55
2:B:1208:ASN:O	2:B:1279:ARG:NH1	2.41	0.54
2:B:977:GLU:HG3	2:B:1310:ILE:HG23	1.89	0.53
2:B:1148:LYS:NZ	2:B:1189:GLU:OE1	2.41	0.53
2:B:1216:SER:OG	4:D:7:DC:OP1	2.23	0.53
4:D:9:DA:H4'	4:D:10:DT:OP1	2.10	0.52
1:A:18:A:OP1	2:B:165:ARG:HD3	2.09	0.51
2:B:225:LEU:HD23	2:B:242:ILE:HG21	1.91	0.51
2:B:910:GLU:HG2	2:B:1033:THR:HG23	1.93	0.51
2:B:497:ASN:HD21	3:C:19:DA:P	2.33	0.51
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.93	0.51
4:D:6:DG:H2''	4:D:7:DC:H5'	1.92	0.50
4:D:9:DA:H2''	4:D:10:DT:H5'	1.93	0.50
2:B:746:GLU:OE2	2:B:1351:SER:HB3	2.10	0.50
3:C:19:DA:H5''	3:C:19:DA:H8	1.76	0.50
2:B:211:ILE:HD11	2:B:225:LEU:N	2.26	0.49
2:B:1270:ILE:HD12	2:B:1294:TYR:CD2	2.47	0.49
2:B:1117:ASP:N	2:B:1117:ASP:OD1	2.44	0.49
1:A:22:U:H2'	1:A:23:U:C6	2.46	0.49
2:B:699:ASP:OD1	2:B:701:SER:OG	2.26	0.49
2:B:338:LEU:HB3	2:B:383:MET:HE2	1.95	0.49
1:A:73:G:H3'	1:A:74:A:C5'	2.42	0.48
2:B:148:LYS:HD2	2:B:429:PHE:HB3	1.96	0.48
2:B:1122:ARG:HG3	2:B:1134:PHE:CE2	2.49	0.47
4:D:9:DA:H1'	4:D:10:DT:H5'	1.96	0.47
1:A:3:A:H2'	1:A:4:A:C8	2.50	0.47
2:B:780:ARG:NH1	2:B:806:LEU:O	2.45	0.47
2:B:305:ILE:HG21	2:B:410:ILE:HG12	1.96	0.47
2:B:161:MET:CE	2:B:419:LEU:N	2.78	0.46
2:B:212:LEU:O	2:B:221:ARG:NE	2.48	0.46
3:C:8:DA:H4'	3:C:9:DT:OP2	2.14	0.46
2:B:1060:ARG:NH1	2:B:1064:GLU:OE1	2.49	0.46
1:A:27:G:H4'	1:A:28:A:OP2	2.14	0.46
2:B:1284:ASP:OD1	2:B:1284:ASP:N	2.49	0.45
2:B:247:GLY:O	7:B:2019:HOH:O	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:LEU:O	2:B:226:ILE:HG22	2.16	0.45
2:B:216:LEU:O	2:B:221:ARG:NH1	2.50	0.45
1:A:68:A:C4	1:A:69:A:C8	3.04	0.45
1:A:54:G:H2'	1:A:55:C:C6	2.52	0.45
2:B:870:VAL:HG13	2:B:871:PRO:HD2	1.98	0.44
2:B:817:GLN:O	2:B:882:TYR:OH	2.36	0.44
2:B:323:LYS:O	2:B:327:GLU:HG3	2.18	0.44
1:A:8:A:H2'	1:A:9:A:C8	2.53	0.44
2:B:122:ILE:H	2:B:122:ILE:HD12	1.83	0.44
2:B:1091:GLN:O	2:B:1091:GLN:HG3	2.17	0.44
1:A:42:A:O2'	1:A:43:G:P	2.76	0.44
2:B:597:LEU:O	2:B:601:ILE:HB	2.16	0.44
2:B:161:MET:HE2	2:B:419:LEU:HB2	1.99	0.43
2:B:1207:GLU:HB2	2:B:1208:ASN:H	1.65	0.43
3:C:7:DC:H2''	3:C:8:DA:C8	2.54	0.43
2:B:307:ARG:NH2	2:B:397:ASP:OD2	2.51	0.43
2:B:629:ARG:NE	2:B:653:ARG:HA	2.34	0.43
2:B:386:THR:O	2:B:386:THR:HG22	2.19	0.43
2:B:356:LYS:O	2:B:357:ASN:HB2	2.19	0.43
2:B:623:LEU:HG	2:B:654:ARG:O	2.19	0.43
1:A:30:C:H2'	1:A:31:U:C6	2.53	0.42
1:A:37:U:H2'	1:A:38:A:H5''	2.01	0.42
2:B:5:TYR:CE1	2:B:751:MET:HG2	2.54	0.42
1:A:75:A:H2'	1:A:76:A:C8	2.54	0.42
2:B:1252:ASN:O	2:B:1255:LYS:HG3	2.19	0.42
2:B:962:LEU:HD22	2:B:1043:MET:SD	2.59	0.42
4:D:9:DA:H1'	4:D:10:DT:C5'	2.50	0.42
2:B:345:GLU:OE1	2:B:345:GLU:N	2.42	0.42
2:B:584:GLU:O	2:B:586:ARG:N	2.51	0.42
2:B:1052:LEU:O	7:B:2072:HOH:O	2.21	0.42
2:B:1205:GLU:HG3	2:B:1211:LYS:HG2	2.02	0.42
3:C:17:DA:H2'	3:C:18:DA:C8	2.55	0.42
2:B:1204:PHE:CD1	2:B:1342:VAL:HG13	2.54	0.42
2:B:215:ARG:HG3	2:B:307:ARG:NE	2.34	0.42
1:A:48:A:H2'	1:A:49:A:C8	2.55	0.42
2:B:248:LEU:HD23	2:B:249:THR:H	1.85	0.41
2:B:343:LEU:HD11	2:B:383:MET:SD	2.59	0.41
1:A:46:A:H2'	1:A:47:A:C8	2.55	0.41
1:A:61:C:OP2	2:B:70:ARG:HD3	2.20	0.41
1:A:71:U:H2'	1:A:72:U:H5'	2.02	0.41
2:B:212:LEU:HD12	2:B:246:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:LEU:HD11	2:B:225:LEU:HD22	2.01	0.41
2:B:222:LEU:O	2:B:223:GLU:C	2.62	0.41
2:B:226:ILE:HG13	2:B:226:ILE:O	2.21	0.41
2:B:446:PHE:CG	2:B:447:ARG:N	2.88	0.41
3:C:19:DA:H2'	3:C:20:DT:H71	2.01	0.41
2:B:802:GLU:O	2:B:803:ASN:C	2.63	0.41
2:B:1270:ILE:O	2:B:1271:GLU:C	2.60	0.41
1:A:74:A:C2'	1:A:75:A:H5'	2.51	0.41
2:B:45:LYS:HA	2:B:1091:GLN:OE1	2.21	0.41
2:B:790:GLU:HG2	2:B:889:ALA:HA	2.03	0.41
2:B:1146:VAL:HG11	2:B:1194:LEU:HD12	2.03	0.41
2:B:1200:LYS:HE2	2:B:1201:TYR:CZ	2.55	0.41
1:A:42:A:C5'	1:A:42:A:H8	2.34	0.41
2:B:827:GLU:O	2:B:859:ARG:NH2	2.45	0.41
2:B:398:LEU:HG	2:B:399:LEU:HG	2.03	0.41
2:B:1119:LEU:HB3	2:B:1128:PRO:HB2	2.02	0.41
2:B:211:ILE:O	2:B:211:ILE:HG13	2.22	0.40
1:A:42:A:O2'	1:A:43:G:H5'	2.22	0.40
2:B:15:SER:HA	2:B:51:LEU:O	2.21	0.40
2:B:450:TYR:OH	2:B:627:GLU:HG2	2.21	0.40
2:B:665:LYS:HA	2:B:669:GLY:HA3	2.03	0.40
2:B:612:ASN:O	2:B:613:GLU:C	2.65	0.40
2:B:1256:GLN:NE2	2:B:1260:GLU:OE1	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:571:LYS:NZ	2:B:825:ASP:OD2[4_758]	2.19	0.01

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	
2	B	1310/1372 (96%)	1254 (96%)	56 (4%)	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	
2	B	1188/1227 (97%)	1033 (87%)	155 (13%)	4	10

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	23	ASP
2	B	27	VAL
2	B	29	SER
2	B	31	LYS
2	B	39	ASP
2	B	44	LYS
2	B	64	LEU
2	B	73	THR
2	B	82	LEU
2	B	101	LEU
2	B	106	LEU
2	B	122	ILE
2	B	123	VAL
2	B	139	ARG
2	B	141	LYS
2	B	161	MET
2	B	165	ARG
2	B	173	ASP
2	B	174	LEU
2	B	178	ASN
2	B	188	LEU
2	B	195	LEU
2	B	198	GLU

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Mol	Chain	Res	Type
2	B	204	SER
2	B	211	ILE
2	B	212	LEU
2	B	215	ARG
2	B	219	SER
2	B	220	ARG
2	B	226	ILE
2	B	234	LYS
2	B	244	LEU
2	B	248	LEU
2	B	263	LYS
2	B	268	LYS
2	B	300	ILE
2	B	305	ILE
2	B	311	GLU
2	B	313	THR
2	B	334	LEU
2	B	343	LEU
2	B	377	LYS
2	B	384	ASP
2	B	403	ARG
2	B	409	SER
2	B	419	LEU
2	B	424	ARG
2	B	438	GLU
2	B	445	THR
2	B	455	LEU
2	B	510	LYS
2	B	514	LEU
2	B	534	MET
2	B	536	LYS
2	B	540	LEU
2	B	557	ARG
2	B	579	GLU
2	B	583	VAL
2	B	584	GLU
2	B	598	LEU
2	B	599	LYS
2	B	601	ILE
2	B	602	LYS
2	B	623	LEU
2	B	627	GLU

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Mol	Chain	Res	Type
2	B	630	GLU
2	B	635	ARG
2	B	637	LYS
2	B	638	THR
2	B	643	PHE
2	B	661	ARG
2	B	666	LEU
2	B	675	SER
2	B	694	MET
2	B	696	LEU
2	B	697	ILE
2	B	709	GLN
2	B	738	LEU
2	B	750	VAL
2	B	751	MET
2	B	765	ARG
2	B	776	ASN
2	B	778	ARG
2	B	781	MET
2	B	782	LYS
2	B	783	ARG
2	B	785	GLU
2	B	790	GLU
2	B	794	GLN
2	B	796	LEU
2	B	798	GLU
2	B	801	VAL
2	B	811	LEU
2	B	827	GLU
2	B	830	ILE
2	B	832	ARG
2	B	842	VAL
2	B	856	VAL
2	B	866	LYS
2	B	867	SER
2	B	868	ASP
2	B	878	LYS
2	B	884	ARG
2	B	887	LEU
2	B	918	LYS
2	B	919	ARG
2	B	921	LEU

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Mol	Chain	Res	Type
2	B	935	LEU
2	B	945	GLU
2	B	948	LYS
2	B	952	GLU
2	B	957	THR
2	B	959	LYS
2	B	968	LYS
2	B	977	GLU
2	B	998	ILE
2	B	1003	LYS
2	B	1007	GLU
2	B	1028	GLU
2	B	1029	ILE
2	B	1031	LYS
2	B	1033	THR
2	B	1035	LYS
2	B	1048	THR
2	B	1049	GLU
2	B	1057	ILE
2	B	1087	LEU
2	B	1091	GLN
2	B	1114	ARG
2	B	1116	SER
2	B	1117	ASP
2	B	1122	ARG
2	B	1135	VAL
2	B	1136	SER
2	B	1138	THR
2	B	1146	VAL
2	B	1148	LYS
2	B	1151	LYS
2	B	1160	VAL
2	B	1175	GLU
2	B	1191	LYS
2	B	1206	LEU
2	B	1207	GLU
2	B	1214	LEU
2	B	1218	ARG
2	B	1240	SER
2	B	1266	LEU
2	B	1270	ILE
2	B	1275	GLU

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Mol	Chain	Res	Type
2	B	1304	GLU
2	B	1314	THR
2	B	1325	LYS
2	B	1351	SER
2	B	1363	SER
2	B	1365	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	175	ASN
2	B	199	ASN
2	B	497	ASN
2	B	501	ASN
2	B	556	ASN
2	B	712	GLN
2	B	799	HIS
2	B	805	GLN
2	B	818	ASN
2	B	831	ASN
2	B	885	GLN
2	B	894	GLN
2	B	946	ASN
2	B	1093	ASN
2	B	1101	GLN
2	B	1264	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	80/83 (96%)	22 (27%)	4 (5%)

All (22) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	A
1	A	20	A
1	A	24	U
1	A	28	A
1	A	29	G

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Mol	Chain	Res	Type
1	A	31	U
1	A	32	A
1	A	35	A
1	A	37	U
1	A	38	A
1	A	39	G
1	A	40	C
1	A	42	A
1	A	43	G
1	A	44	U
1	A	51	A
1	A	56	U
1	A	59	U
1	A	68	A
1	A	74	A
1	A	75	A
1	A	78	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	27	G
1	A	28	A
1	A	42	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

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

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 [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	81/83 (97%)	-0.23	2 (2%) 58 55	24, 48, 123, 158	0
2	B	1322/1372 (96%)	0.28	55 (4%) 40 37	21, 58, 101, 161	0
3	C	28/28 (100%)	-0.16	0 100 100	32, 51, 81, 114	0
4	D	11/12 (91%)	0.84	1 (9%) 15 12	41, 75, 123, 125	0
All	All	1442/1495 (96%)	0.25	58 (4%) 42 38	21, 57, 103, 161	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	2	DA	4.8
2	B	178	ASN	4.6
2	B	1241	HIS	4.3
2	B	776	ASN	4.1
2	B	721	HIS	3.5
2	B	199	ASN	3.5
2	B	1052	LEU	3.4
2	B	3	LYS	3.3
2	B	204	SER	3.3
2	B	302	LEU	3.3
2	B	718	ASP	3.2
2	B	203	ALA	3.2
2	B	248	LEU	3.0
2	B	868	ASP	3.0
2	B	289	LEU	3.0
2	B	584	GLU	2.9
2	B	862	LYS	2.9
2	B	1115	ASN	2.9
2	B	1053	ALA	2.8
2	B	242	ILE	2.8
2	B	1215	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	1077	GLY	2.7
2	B	205	GLY	2.6
2	B	294	LYS	2.6
2	B	1252	ASN	2.6
2	B	661	ARG	2.5
2	B	102	GLU	2.5
2	B	1216	SER	2.4
1	A	77	A	2.4
2	B	246	LEU	2.4
2	B	197	GLU	2.4
2	B	1117	ASP	2.4
2	B	262	ALA	2.4
2	B	1207	GLU	2.4
2	B	181	VAL	2.4
2	B	1298	ARG	2.3
2	B	1029	ILE	2.3
2	B	688	PHE	2.3
2	B	292	ALA	2.3
2	B	1116	SER	2.3
2	B	259	ALA	2.2
2	B	826	GLN	2.2
2	B	311	GLU	2.2
2	B	268	LYS	2.2
2	B	385	GLY	2.2
2	B	766	GLU	2.1
2	B	1326	TYR	2.1
2	B	274	ASP	2.1
2	B	976	ARG	2.1
2	B	581	SER	2.1
2	B	200	PRO	2.1
2	B	269	ASP	2.1
1	A	78	A	2.1
2	B	711	ALA	2.0
2	B	225	LEU	2.0
2	B	712	GLN	2.0
2	B	907	GLY	2.0
2	B	215	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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 [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, 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
6	K	B	2371	1/1	0.75	0.13	60,60,60,60	0
6	K	A	1183	1/1	0.82	0.13	59,59,59,59	0
6	K	B	2374	1/1	0.82	0.09	61,61,61,61	0
6	K	A	1182	1/1	0.92	0.10	60,60,60,60	0
6	K	B	2370	1/1	0.92	0.09	59,59,59,59	0
6	K	B	2373	1/1	0.94	0.07	62,62,62,62	0
6	K	B	2372	1/1	0.95	0.09	61,61,61,61	0
6	K	B	2367	1/1	0.96	0.07	53,53,53,53	0
6	K	B	2369	1/1	0.97	0.06	45,45,45,45	0
6	K	B	2366	1/1	0.97	0.04	46,46,46,46	0
6	K	B	2368	1/1	0.98	0.05	41,41,41,41	0
5	MG	A	1084	1/1	0.99	0.09	32,32,32,32	0
5	MG	A	1083	1/1	0.99	0.08	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.