



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 11:23 AM UTC

PDB ID : 5B2P / pdb\_00005b2p  
Title : Crystal structure of Francisella novicida Cas9 in complex with sgRNA and target DNA (TGA PAM)  
Authors : Hirano, H.; Nishimasu, H.; Nakane, T.; Ishitani, R.; Nureki, O.  
Deposited on : 2016-02-01  
Resolution : 1.70 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

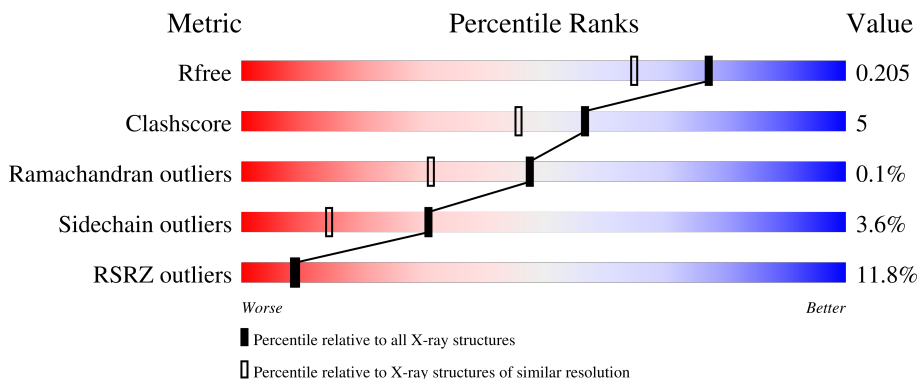
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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  $\geq 3$ , 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	1632	
2	B	94	
3	C	30	
4	D	9	

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 15757 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 Cas9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1455	11809	7555	2030	2193	31	0	18	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0Q5Y3
A	-1	SER	-	expression tag	UNP A0Q5Y3
A	0	HIS	-	expression tag	UNP A0Q5Y3
A	995	ALA	ASN	engineered mutation	UNP A0Q5Y3

- Molecule 2 is DNA/RNA hybrid called Guide RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	94	1991	886	350	661	94	0	0	0

- Molecule 3 is a DNA chain called Target DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	30	596	286	104	177	29	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(\*TP\*GP\*AP\*TP\*AP\*TP\*CP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	D	9	184	89	34	53	8	0	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

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

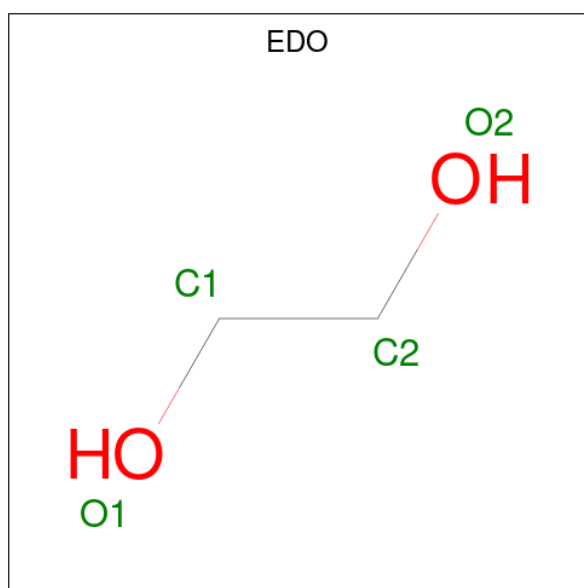
- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Cl 2 2	0	0

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	11	Total Ca 11 11	0	0
8	B	6	Total Ca 6 6	0	0

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



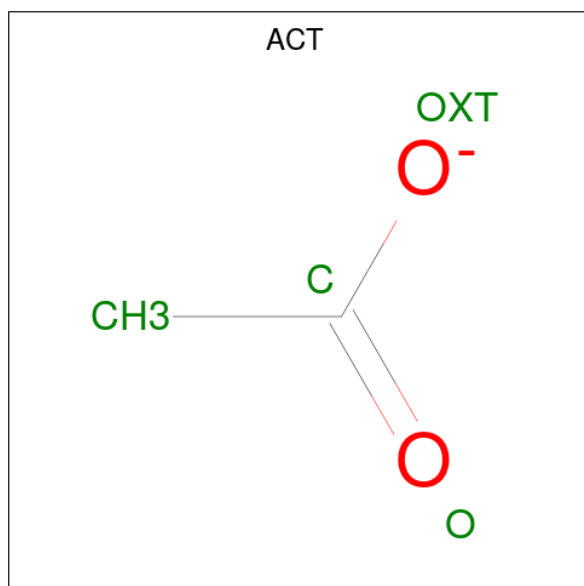
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

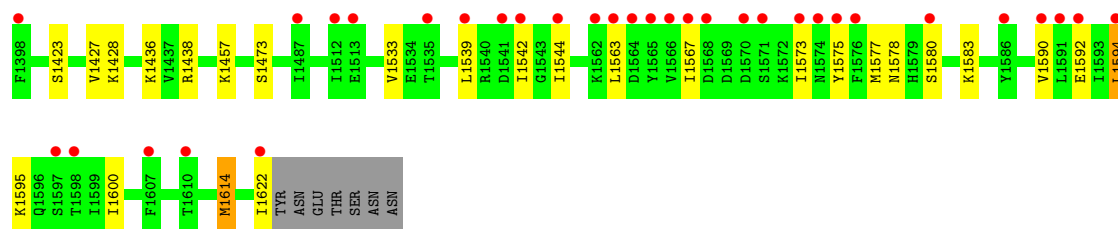


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		

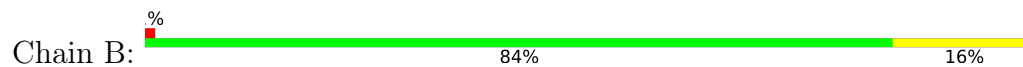
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	639	Total	O	0	0
			639	639		
11	B	342	Total	O	0	0
			342	342		
11	C	68	Total	O	0	0
			68	68		
11	D	4	Total	O	0	0
			4	4		





- Molecule 2: Guide RNA



- Molecule 3: Target DNA



- Molecule 4: DNA (5'-D(\*TP\*GP\*AP\*TP\*AP\*TP\*CP\*GP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.61Å 159.27Å 96.67Å 90.00° 106.86° 90.00°	Depositor
Resolution (Å)	46.26 – 1.70 46.26 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.26-1.70) 98.7 (46.26-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 1.70Å)	Xtrriage
Refinement program	PHENIX 1.10_2155: ???	Depositor
R, $R_{free}$	0.180 , 0.203 0.183 , 0.205	Depositor DCC
$R_{free}$ test set	12766 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtrriage
Anisotropy	0.036	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15757	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: ZN, CL, EDO, CA, NA, ACT

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	0.62	0/12080	0.71	3/16292 (0.0%)
2	B	0.87	0/2224	0.89	2/3465 (0.1%)
3	C	0.77	0/665	0.91	0/1020
4	D	0.56	0/206	0.63	0/317
All	All	0.67	0/15175	0.75	5/21094 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	310	ARG	CG-CD-NE	-7.32	95.91	112.00
2	B	34	C	C5'-C4'-C3'	-6.38	106.42	116.00
2	B	33	G	O3'-P-O5'	-5.49	95.77	104.00
1	A	1397	PRO	CA-C-N	-5.46	112.49	122.38
1	A	1397	PRO	C-N-CA	-5.46	112.49	122.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	36	G	Sidechain

## 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	11809	0	11590	107	0
2	B	1991	0	997	14	0
3	C	596	0	338	12	0
4	D	184	0	104	2	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	2	0	0	0	0
8	A	11	0	0	0	0
8	B	6	0	0	0	0
9	A	44	0	66	3	0
9	B	44	0	66	8	0
9	C	4	0	6	0	0
10	A	4	0	3	0	0
10	B	4	0	3	0	0
11	A	639	0	0	13	0
11	B	342	0	0	2	0
11	C	68	0	0	0	0
11	D	4	0	0	0	0
All	All	15757	0	13173	127	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 5.

The worst 5 of 127 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:54[B]:ASN:OD1	1:A:58[B]:ARG:NH1	1.91	1.03
1:A:169:LYS:HB3	1:A:187:LEU:HD21	1.63	0.79
3:C:22:DT:H5''	3:C:22:DT:H6	1.46	0.79
1:A:906:PRO:HA	1:A:916:LEU:HD21	1.64	0.78
1:A:578:LYS:NZ	1:A:582:GLU:OE2	2.17	0.77

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	1445/1632 (88%)	1407 (97%)	37 (3%)	1 (0%)	48 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1128	GLY

### 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	1259/1484 (85%)	1214 (96%)	45 (4%)	31 14

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	987	LEU
1	A	1428	LYS
1	A	1088	VAL
1	A	1302	ILE
1	A	1563	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1051	ASN
1	A	1157	GLN
1	A	1504	ASN
1	A	1234	ASN
1	A	1129	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 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 49 ligands modelled in this entry, 24 are monoatomic - leaving 25 for Mogul analysis.

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
9	EDO	A	1722	-	3,3,3	0.40	0	2,2,2	0.74	0
10	ACT	A	1728	-	3,3,3	0.42	0	3,3,3	1.32	0
9	EDO	C	101	-	3,3,3	0.56	0	2,2,2	0.20	0
9	EDO	A	1717	-	3,3,3	0.35	0	2,2,2	0.78	0
9	EDO	A	1723	-	3,3,3	0.63	0	2,2,2	0.35	0
9	EDO	A	1718	-	3,3,3	0.47	0	2,2,2	0.75	0
9	EDO	B	119	-	3,3,3	0.46	0	2,2,2	0.22	0
9	EDO	B	113	-	3,3,3	0.48	0	2,2,2	0.31	0
9	EDO	B	118	-	3,3,3	0.34	0	2,2,2	0.39	0
9	EDO	A	1727	-	3,3,3	0.38	0	2,2,2	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	EDO	B	110	-	3,3,3	0.65	0	2,2,2	0.78	0
9	EDO	A	1719	-	3,3,3	0.60	0	2,2,2	0.34	0
9	EDO	B	117	-	3,3,3	0.54	0	2,2,2	0.35	0
9	EDO	A	1726	-	3,3,3	0.45	0	2,2,2	0.33	0
9	EDO	B	111	-	3,3,3	0.64	0	2,2,2	0.19	0
9	EDO	B	115	-	3,3,3	0.58	0	2,2,2	0.14	0
9	EDO	B	116	-	3,3,3	0.37	0	2,2,2	0.71	0
9	EDO	B	112	-	3,3,3	0.81	0	2,2,2	0.13	0
9	EDO	A	1725	-	3,3,3	0.59	0	2,2,2	0.22	0
9	EDO	A	1721	-	3,3,3	0.75	0	2,2,2	0.71	0
9	EDO	A	1720	-	3,3,3	1.02	0	2,2,2	0.20	0
9	EDO	B	109	-	3,3,3	0.55	0	2,2,2	0.47	0
9	EDO	A	1724	-	3,3,3	0.57	0	2,2,2	0.14	0
9	EDO	B	114	-	3,3,3	0.72	0	2,2,2	0.30	0
10	ACT	B	120	-	3,3,3	0.82	0	3,3,3	1.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	1722	-	-	1/1/1/1	-
9	EDO	C	101	-	-	0/1/1/1	-
9	EDO	A	1717	-	-	1/1/1/1	-
9	EDO	A	1723	-	-	0/1/1/1	-
9	EDO	A	1718	-	-	0/1/1/1	-
9	EDO	B	119	-	-	0/1/1/1	-
9	EDO	B	113	-	-	0/1/1/1	-
9	EDO	B	118	-	-	0/1/1/1	-
9	EDO	A	1727	-	-	0/1/1/1	-
9	EDO	B	110	-	-	1/1/1/1	-
9	EDO	A	1719	-	-	0/1/1/1	-
9	EDO	B	117	-	-	1/1/1/1	-
9	EDO	A	1726	-	-	0/1/1/1	-
9	EDO	B	111	-	-	0/1/1/1	-
9	EDO	B	115	-	-	1/1/1/1	-
9	EDO	B	116	-	-	0/1/1/1	-
9	EDO	B	112	-	-	0/1/1/1	-
9	EDO	A	1725	-	-	1/1/1/1	-
9	EDO	A	1721	-	-	0/1/1/1	-
9	EDO	A	1720	-	-	0/1/1/1	-
9	EDO	B	109	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	1724	-	-	0/1/1/1	-
9	EDO	B	114	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1725	EDO	O1-C1-C2-O2
9	B	110	EDO	O1-C1-C2-O2
9	B	117	EDO	O1-C1-C2-O2
9	A	1722	EDO	O1-C1-C2-O2
9	B	115	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1722	EDO	2	0
9	B	119	EDO	1	0
9	B	118	EDO	3	0
9	B	117	EDO	1	0
9	A	1726	EDO	1	0
9	B	116	EDO	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

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, 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	1455/1632 (89%)	0.71	186 (12%) 7 7	13, 44, 95, 129	18 (1%)
2	B	94/94 (100%)	-0.49	1 (1%) 78 81	20, 30, 59, 80	0
3	C	30/30 (100%)	0.17	1 (3%) 49 53	24, 46, 92, 133	0
4	D	9/9 (100%)	0.76	0 100 100	39, 52, 111, 119	0
All	All	1588/1765 (89%)	0.63	188 (11%) 9 9	13, 43, 94, 133	18 (1%)

The worst 5 of 188 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	VAL	6.7
1	A	1567	ILE	6.3
1	A	1072	ILE	5.8
1	A	1542	ILE	4.7
1	A	759	TYR	4.6

### 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 [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
9	EDO	B	118	4/4	0.79	0.21	56,57,58,58	0
6	NA	A	1703	1/1	0.81	0.12	61,61,61,61	0
9	EDO	A	1727	4/4	0.82	0.22	62,62,63,65	0
9	EDO	A	1725	4/4	0.83	0.15	60,61,61,62	0
8	CA	A	1713	1/1	0.84	0.11	96,96,96,96	0
10	ACT	B	120	4/4	0.85	0.22	76,77,77,77	0
9	EDO	A	1722	4/4	0.88	0.17	48,49,52,53	0
9	EDO	B	114	4/4	0.89	0.16	46,49,52,52	0
9	EDO	B	117	4/4	0.89	0.15	43,45,46,46	0
9	EDO	B	119	4/4	0.90	0.13	44,46,47,49	0
9	EDO	A	1724	4/4	0.91	0.12	44,45,45,46	0
9	EDO	A	1718	4/4	0.91	0.12	36,40,43,48	0
9	EDO	A	1721	4/4	0.92	0.15	32,32,36,36	0
8	CA	B	108	1/1	0.92	0.18	80,80,80,80	0
9	EDO	C	101	4/4	0.92	0.13	45,49,50,52	0
9	EDO	A	1726	4/4	0.92	0.11	49,49,56,58	0
9	EDO	B	115	4/4	0.93	0.12	43,47,52,55	0
9	EDO	B	116	4/4	0.93	0.13	37,47,50,51	0
8	CA	B	104	1/1	0.93	0.08	73,73,73,73	0
8	CA	B	106	1/1	0.93	0.13	54,54,54,54	0
8	CA	B	107	1/1	0.93	0.11	84,84,84,84	0
9	EDO	B	113	4/4	0.93	0.12	36,36,39,40	0
8	CA	A	1711	1/1	0.93	0.08	79,79,79,79	0
9	EDO	A	1720	4/4	0.94	0.11	30,36,38,39	0
9	EDO	A	1717	4/4	0.95	0.10	40,42,44,45	0
8	CA	A	1714	1/1	0.95	0.10	60,60,60,60	0
8	CA	A	1709	1/1	0.95	0.13	50,50,50,50	0
6	NA	A	1702	1/1	0.95	0.11	43,43,43,43	0
8	CA	A	1712	1/1	0.95	0.11	61,61,61,61	0
6	NA	B	102	1/1	0.95	0.12	46,46,46,46	0
8	CA	A	1706	1/1	0.96	0.08	67,67,67,67	0
8	CA	A	1710	1/1	0.96	0.15	48,48,48,48	0
8	CA	A	1716	1/1	0.96	0.15	56,56,56,56	0
9	EDO	A	1719	4/4	0.96	0.07	31,34,37,39	0
9	EDO	B	112	4/4	0.97	0.07	28,29,32,32	0
7	CL	A	1704	1/1	0.97	0.09	43,43,43,43	0
9	EDO	A	1723	4/4	0.97	0.10	27,32,37,42	0
9	EDO	B	109	4/4	0.97	0.07	30,31,33,36	0
10	ACT	A	1728	4/4	0.97	0.07	32,33,34,35	0
9	EDO	B	110	4/4	0.97	0.07	32,33,33,37	0
8	CA	A	1715	1/1	0.98	0.19	52,52,52,52	0
8	CA	A	1708	1/1	0.98	0.12	42,42,42,42	0
9	EDO	B	111	4/4	0.99	0.05	23,24,24,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ZN	A	1701	1/1	0.99	0.02	26,26,26,26	0
8	CA	B	103	1/1	0.99	0.06	33,33,33,33	0
6	NA	B	101	1/1	0.99	0.04	27,27,27,27	0
8	CA	B	105	1/1	0.99	0.03	35,35,35,35	0
7	CL	A	1705	1/1	0.99	0.08	28,28,28,28	0
8	CA	A	1707	1/1	1.00	0.10	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.