



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:19 PM UTC

PDB ID : 5B2O / pdb_00005b2o
Title : Crystal structure of Francisella novicida Cas9 in complex with sgRNA and target DNA (TGG 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 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

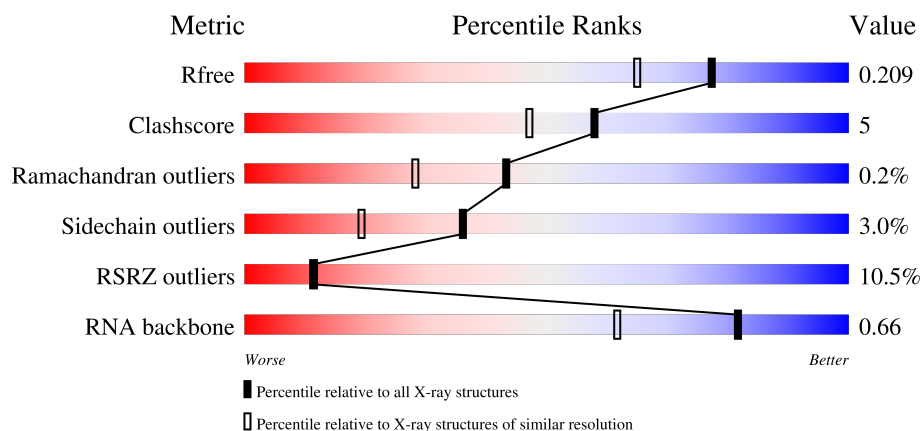
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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)
RNA backbone	3983	1094 (2.20-1.20)

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	1632	10% 79% 10% 11%
2	B	94	2% 76% 21%
3	C	30	63% 37%
4	D	9	78% 22%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15717 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
1	A	1455	Total	C	N	O	S	0	19	0
			11791	7536	2025	2199	31			

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 a RNA chain called Guide RNA.

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

- Molecule 3 is a DNA chain called Target DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	30	Total	C	N	O	P	0	0	0
			595	285	105	176	29			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	9	Total	C	N	O	P	0	0	0
			185	89	34	54	8			

- 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

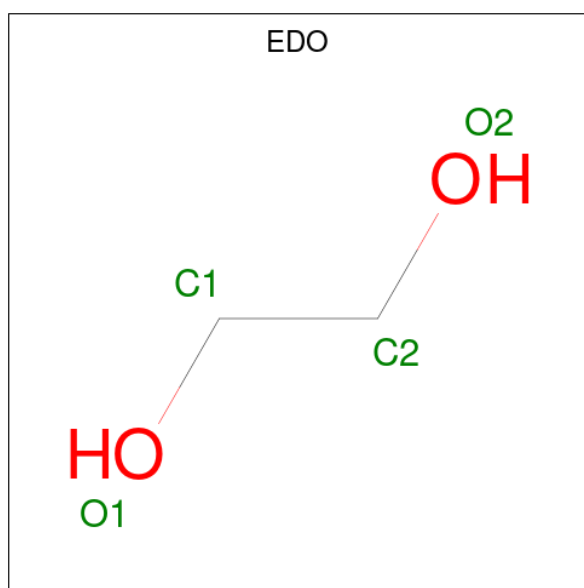
- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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	10	Total Ca 10 10	0	0
8	B	7	Total Ca 7 7	0	0

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



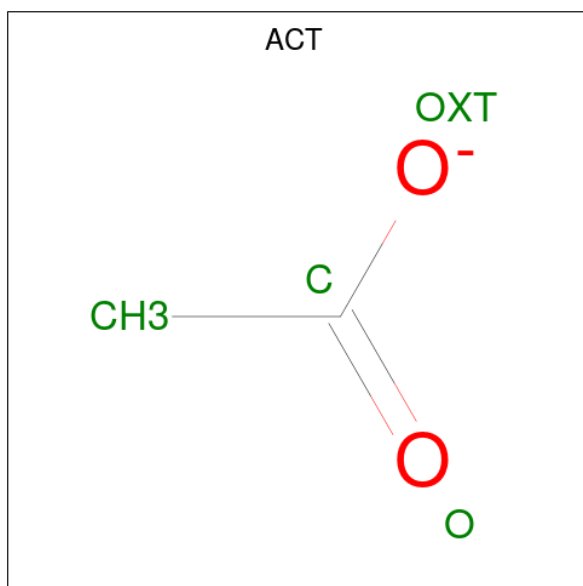
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0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

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

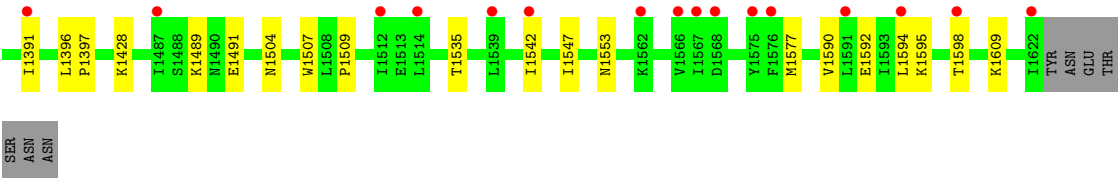
- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



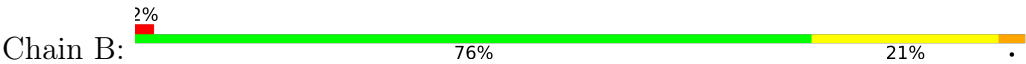
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	618	Total	O	0	0
			618	618		
11	B	334	Total	O	0	0
			334	334		
11	C	71	Total	O	0	0
			71	71		
11	D	8	Total	O	0	0
			8	8		



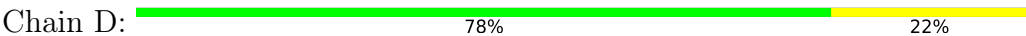
● Molecule 2: Guide RNA



● Molecule 3: Target DNA



● Molecule 4: DNA (5'-D(*TP*GP*GP*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, α , β , γ	81.92Å 159.10Å 96.81Å 90.00° 107.04° 90.00°	Depositor
Resolution (Å)	46.28 – 1.70 46.28 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.2 (46.28-1.70) 96.1 (46.28-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.10_2155: ???	Depositor
R, R_{free}	0.184 , 0.207 0.186 , 0.209	Depositor DCC
R_{free} test set	12436 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15717	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, CA, EDO, ZN, NA, CL

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	0.44	0/12068	0.59	3/16282 (0.0%)
2	B	0.62	1/2224 (0.0%)	0.75	0/3465
3	C	0.58	0/664	0.72	0/1018
4	D	0.45	0/207	0.62	0/319
All	All	0.48	1/15163 (0.0%)	0.63	3/21084 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	57	DU	O3'-P	5.48	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ARG	CG-CD-NE	-7.41	95.70	112.00
1	A	1397	PRO	CA-C-N	-5.32	111.31	121.94
1	A	1397	PRO	C-N-CA	-5.32	111.31	121.94

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

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	11791	0	11524	108	1
2	B	1991	0	997	16	0
3	C	595	0	337	9	0
4	D	185	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	10	0	0	0	0
8	B	7	0	0	0	0
9	A	48	0	72	3	0
9	B	40	0	60	6	0
9	C	4	0	6	0	0
10	A	4	0	3	0	0
10	B	4	0	3	0	0
11	A	618	0	0	12	0
11	B	334	0	0	1	0
11	C	71	0	0	0	0
11	D	8	0	0	0	0
All	All	15717	0	13106	126	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 (126) 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	1.99	0.96
1:A:265:ASN:O	1:A:291:LEU:N	2.08	0.87
1:A:906:PRO:HA	1:A:916:LEU:HD21	1.64	0.80
1:A:1335[A]:GLN:NE2	11:A:1801:HOH:O	2.05	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:DA:H2''	3:C:5:DT:H5''	1.67	0.76
1:A:734:THR:HG21	1:A:738:CYS:H	1.50	0.75
1:A:648[B]:ASP:OD2	1:A:1104:TYR:OH	2.05	0.74
1:A:1292[B]:CYS:HB2	1:A:1332:LEU:HD21	1.72	0.72
1:A:902:PHE:HA	1:A:924:LEU:HD12	1.71	0.72
1:A:58[A]:ARG:NH2	11:A:1805:HOH:O	2.24	0.70
1:A:782:GLU:OE2	1:A:785:ARG:NH2	2.17	0.70
1:A:1326:GLU:HG3	1:A:1327:TYR:CD2	2.27	0.70
1:A:1335[A]:GLN:OE1	11:A:1802:HOH:O	2.10	0.69
1:A:1236:HIS:HE1	11:A:2043:HOH:O	1.77	0.68
1:A:23:PHE:HB2	9:A:1725:EDO:H22	1.74	0.68
1:A:54[B]:ASN:HD21	1:A:58[B]:ARG:CZ	2.06	0.68
3:C:2:DC:H2'	3:C:3:DG:C8	2.30	0.66
1:A:983:ASP:OD2	1:A:1083:ARG:NH2	2.29	0.66
1:A:463:LEU:HD11	1:A:853:ILE:HG13	1.80	0.63
1:A:1609:LYS:N	3:C:3:DG:OP2	2.27	0.63
1:A:981:LEU:HD12	1:A:1080:ILE:HG21	1.81	0.62
1:A:983:ASP:OD1	1:A:984:GLU:N	2.33	0.62
1:A:828:ILE:HG12	1:A:846:LYS:HG3	1.82	0.62
1:A:983:ASP:CG	1:A:1083:ARG:HH22	2.09	0.60
11:A:2330:HOH:O	9:B:116:EDO:H12	2.02	0.60
1:A:693:LEU:HG	1:A:697:LYS:HE3	1.85	0.59
1:A:1302:ILE:HG22	1:A:1304:ILE:HG12	1.85	0.58
1:A:734:THR:CG2	1:A:738:CYS:H	2.16	0.58
2:B:94:G:C2	9:B:117:EDO:H11	2.39	0.57
1:A:159:ASN:ND2	1:A:193:TYR:OH	2.38	0.56
1:A:1577:MET:HE1	1:A:1590:VAL:HG12	1.88	0.56
1:A:648[A]:ASP:OD2	1:A:1104:TYR:OH	2.25	0.55
1:A:1159:SER:OG	1:A:1221:ASP:OD1	2.20	0.55
1:A:145:LYS:O	1:A:148:THR:OG1	2.26	0.55
1:A:791:ASN:H	1:A:791:ASN:HD22	1.55	0.54
1:A:718:LYS:HB2	2:B:9:A:H5'	1.88	0.54
1:A:725:ASN:ND2	1:A:794:TYR:HE2	2.06	0.54
1:A:640:LYS:HE2	1:A:642:ASN:HD21	1.72	0.54
1:A:52:MET:HE3	1:A:864:LYS:HE2	1.90	0.54
3:C:4:DA:C2'	3:C:5:DT:H5''	2.37	0.53
1:A:724:LEU:HD12	1:A:794:TYR:CZ	2.43	0.53
1:A:1489:LYS:HB2	1:A:1491:GLU:HG2	1.90	0.53
2:B:66:U:H4'	2:B:67:U:O5'	2.08	0.53
1:A:174:CYS:HA	1:A:247:ASN:HD21	1.73	0.53
1:A:730:ILE:O	1:A:734:THR:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:DC:O2	4:D:9:DG:N2	2.29	0.52
3:C:24:DA:H5''	3:C:24:DA:H8	1.75	0.52
1:A:1391:ILE:HG12	1:A:1396:LEU:HD11	1.92	0.51
1:A:663[B]:GLN:HA	1:A:810:ASN:HA	1.93	0.51
1:A:698:TRP:CH2	1:A:770:LEU:HD23	2.45	0.51
1:A:1326:GLU:HG3	1:A:1327:TYR:HD2	1.73	0.51
1:A:1070:ASN:OD1	1:A:1072:ILE:HG12	2.12	0.50
1:A:249:ARG:HG2	1:A:249:ARG:HH11	1.77	0.50
3:C:11:DC:H2'	3:C:12:DC:C6	2.47	0.50
1:A:869:LEU:HD23	1:A:1095[B]:PHE:CE1	2.47	0.50
1:A:1504:ASN:ND2	11:A:1804:HOH:O	2.14	0.50
1:A:544[B]:ARG:NH1	1:A:549:ASP:OD1	2.44	0.50
1:A:659:HIS:HD2	11:B:241:HOH:O	1.94	0.50
1:A:423[A]:GLU:CD	1:A:444:ARG:HH22	2.21	0.48
1:A:61[A]:GLN:HG3	11:A:2395:HOH:O	2.12	0.48
1:A:1507:TRP:CD1	1:A:1509:PRO:HD2	2.49	0.48
1:A:12:LEU:HD11	1:A:1095[A]:PHE:CE2	2.47	0.48
1:A:52:MET:SD	9:B:116:EDO:H22	2.53	0.48
1:A:710:CYS:HB3	1:A:800:GLN:HB2	1.95	0.48
1:A:641:TYR:CE2	1:A:1109:LYS:HG2	2.49	0.47
2:B:89:C:H4'	9:B:119:EDO:H11	1.96	0.47
2:B:66:U:H1'	2:B:67:U:OP2	2.14	0.47
1:A:1326:GLU:HG2	11:A:1867:HOH:O	2.15	0.47
3:C:21:DC:H2'	3:C:22:DT:C6	2.49	0.47
1:A:544[B]:ARG:NH1	1:A:551:LEU:HD22	2.30	0.46
2:B:45:U:H2'	2:B:46:C:C6	2.51	0.46
1:A:1293:LEU:HB3	1:A:1300:ILE:HB	1.98	0.45
1:A:1577:MET:HE2	1:A:1594:LEU:HD23	1.98	0.45
1:A:983:ASP:HA	1:A:1129:ASN:HD22	1.81	0.45
1:A:1535:THR:HG22	1:A:1547:ILE:HG13	1.98	0.45
1:A:1047:ARG:HD2	2:B:1:G:C6	2.51	0.45
1:A:1592:GLU:O	1:A:1595:LYS:HG2	2.17	0.45
1:A:663[B]:GLN:HG3	2:B:81:G:H5''	1.99	0.45
1:A:920:ARG:O	1:A:924:LEU:HD23	2.17	0.44
2:B:64:A:H1'	9:B:116:EDO:H21	2.00	0.44
1:A:17:THR:HG21	1:A:869:LEU:HD21	2.00	0.44
1:A:173:LEU:HD11	1:A:237:GLN:HG3	1.99	0.44
1:A:506:SER:HA	1:A:512:TYR:CZ	2.53	0.44
1:A:1302:ILE:CG2	1:A:1304:ILE:HG12	2.48	0.44
1:A:1131:ARG:NH1	1:A:1176:GLU:OE2	2.51	0.43
1:A:1180:ASP:OD1	1:A:1182:SER:OG	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1374:LYS:HE2	11:A:1926:HOH:O	2.17	0.43
1:A:435:ASP:HA	1:A:438:LEU:HD12	2.00	0.43
1:A:51:LEU:HD11	1:A:912:LYS:HA	2.01	0.43
1:A:249:ARG:HG2	1:A:249:ARG:NH1	2.34	0.43
1:A:1292[A]:CYS:SG	1:A:1360:PHE:HE2	2.41	0.43
2:B:38:A:H2'	2:B:39:A:C8	2.54	0.43
1:A:780:LYS:HE3	1:A:784:ASP:OD1	2.19	0.43
1:A:1272:GLU:HG3	11:A:2337:HOH:O	2.19	0.43
1:A:452:ASN:HA	2:B:89:C:N3	2.33	0.43
1:A:1535:THR:HG23	11:A:1817:HOH:O	2.18	0.42
1:A:920:ARG:HA	1:A:920:ARG:HD2	1.65	0.42
1:A:45:LYS:HB3	1:A:911:VAL:HG12	2.01	0.42
1:A:640:LYS:HE3	2:B:68:U:C6	2.54	0.42
1:A:549:ASP:OD1	1:A:551:LEU:HB2	2.19	0.42
1:A:645:GLY:HA2	9:A:1722:EDO:H11	2.01	0.42
1:A:663[A]:GLN:HG3	2:B:81:G:H5''	2.00	0.42
1:A:1091:THR:O	1:A:1095[A]:PHE:HD1	2.01	0.42
2:B:94:G:C4	9:B:117:EDO:H11	2.54	0.42
1:A:33:LEU:HD13	1:A:1185:LEU:HD21	2.02	0.42
1:A:681:ASN:HA	1:A:684:LYS:HG2	2.01	0.42
1:A:174:CYS:HB3	1:A:251:LEU:HB2	2.01	0.42
1:A:178:LYS:HE3	1:A:178:LYS:HB3	1.89	0.42
1:A:622:ARG:NH2	3:C:30:DC:H4'	2.34	0.42
1:A:21:SER:OG	9:A:1725:EDO:H11	2.19	0.42
1:A:161:LEU:O	1:A:165:ILE:HG22	2.20	0.42
1:A:1553:ASN:HB2	4:D:2:DG:H3'	2.01	0.42
1:A:419:ASP:O	1:A:423[A]:GLU:HG3	2.19	0.41
1:A:514:VAL:O	1:A:529:ASP:HA	2.19	0.41
1:A:720:ASN:HB3	1:A:723:LEU:HD12	2.02	0.41
1:A:161:LEU:HD13	1:A:295:VAL:HG22	2.02	0.41
1:A:722:GLY:C	1:A:724:LEU:H	2.29	0.41
1:A:178:LYS:HD3	1:A:251:LEU:HD23	2.02	0.41
1:A:613:LYS:HG2	11:A:2229:HOH:O	2.20	0.41
1:A:1163:LEU:HG	1:A:1167:MET:HE2	2.03	0.41
1:A:1067:ALA:HB3	1:A:1070:ASN:HB2	2.03	0.40
2:B:25:U:H2'	2:B:26:C:C6	2.56	0.40
1:A:550:GLU:H	1:A:550:GLU:CD	2.29	0.40
1:A:1170:PHE:HD2	1:A:1212:ILE:HD13	1.86	0.40
2:B:34:C:H6	2:B:34:C:H5''	1.86	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)
1:A:249:ARG:NH1	1:A:1260:GLU:OE2[2_445]	2.02	0.18

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	1446/1632 (89%)	1405 (97%)	38 (3%)	3 (0%)	43 28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	722	GLY
1	A	723	LEU
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	1255/1484 (85%)	1218 (97%)	37 (3%)	37 20

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ASP
1	A	137	GLU
1	A	150	GLN

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Mol	Chain	Res	Type
1	A	165	ILE
1	A	213	LYS
1	A	257	ASP
1	A	310	ARG
1	A	334	LYS
1	A	426	GLN
1	A	479	GLN
1	A	551	LEU
1	A	592	ILE
1	A	684	LYS
1	A	723	LEU
1	A	724	LEU
1	A	725	ASN
1	A	730	ILE
1	A	734	THR
1	A	791	ASN
1	A	827	GLN
1	A	828	ILE
1	A	856	ARG
1	A	917	LYS
1	A	932	ILE
1	A	942	GLU
1	A	982	ASN
1	A	1006	ARG
1	A	1048	SER
1	A	1056	GLU
1	A	1083	ARG
1	A	1139	LEU
1	A	1157	GLN
1	A	1234	ASN
1	A	1301	SER
1	A	1428	LYS
1	A	1542	ILE
1	A	1598	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	159	ASN
1	A	247	ASN
1	A	293	HIS

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Mol	Chain	Res	Type
1	A	299	ASN
1	A	317	GLN
1	A	342	ASN
1	A	373	ASN
1	A	426	GLN
1	A	488	GLN
1	A	492	ASN
1	A	554	ASN
1	A	599	ASN
1	A	604	GLN
1	A	642	ASN
1	A	677	GLN
1	A	725	ASN
1	A	761	HIS
1	A	791	ASN
1	A	800	GLN
1	A	827	GLN
1	A	931	ASN
1	A	938	ASN
1	A	1051	ASN
1	A	1157	GLN
1	A	1211	GLN
1	A	1234	ASN
1	A	1236	HIS
1	A	1344	ASN
1	A	1504	ASN
1	A	1554	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	91/94 (96%)	7 (7%)	2 (2%)

All (7) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	18	G
2	B	29	U
2	B	53	C
2	B	67	U
2	B	68	U

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Mol	Chain	Res	Type
2	B	83	U
2	B	84	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	66	U
2	B	67	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](#)

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	0.32	0	2,2,2	0.69	0
9	EDO	A	1726	-	3,3,3	0.49	0	2,2,2	0.16	0
9	EDO	B	116	-	3,3,3	0.37	0	2,2,2	0.59	0
9	EDO	B	111	-	3,3,3	0.61	0	2,2,2	0.33	0
9	EDO	A	1718	-	3,3,3	0.41	0	2,2,2	0.72	0
9	EDO	A	1720	-	3,3,3	0.57	0	2,2,2	0.40	0
10	ACT	B	120	-	3,3,3	0.78	0	3,3,3	1.35	0
9	EDO	B	117	-	3,3,3	0.34	0	2,2,2	0.27	0
9	EDO	A	1724	-	3,3,3	0.50	0	2,2,2	0.06	0
9	EDO	A	1721	-	3,3,3	0.65	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	A	1727	-	3,3,3	0.35	0	2,2,2	0.63	0
9	EDO	A	1716	-	3,3,3	0.39	0	2,2,2	0.43	0
9	EDO	B	110	-	3,3,3	0.39	0	2,2,2	0.50	0
9	EDO	A	1719	-	3,3,3	0.51	0	2,2,2	0.13	0
9	EDO	B	118	-	3,3,3	0.47	0	2,2,2	0.28	0
9	EDO	B	114	-	3,3,3	0.52	0	2,2,2	0.06	0
9	EDO	A	1725	-	3,3,3	0.44	0	2,2,2	0.21	0
10	ACT	A	1728	-	3,3,3	0.83	0	3,3,3	0.99	0
9	EDO	B	113	-	3,3,3	0.79	0	2,2,2	0.18	0
9	EDO	B	119	-	3,3,3	0.42	0	2,2,2	0.39	0
9	EDO	B	115	-	3,3,3	0.47	0	2,2,2	0.15	0
9	EDO	A	1723	-	3,3,3	0.59	0	2,2,2	0.42	0
9	EDO	B	112	-	3,3,3	0.70	0	2,2,2	0.20	0
9	EDO	A	1717	-	3,3,3	0.43	0	2,2,2	0.53	0
9	EDO	C	101	-	3,3,3	0.56	0	2,2,2	0.22	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	A	1726	-	-	1/1/1/1	-
9	EDO	B	116	-	-	0/1/1/1	-
9	EDO	B	111	-	-	1/1/1/1	-
9	EDO	A	1718	-	-	0/1/1/1	-
9	EDO	A	1720	-	-	0/1/1/1	-
9	EDO	B	117	-	-	0/1/1/1	-
9	EDO	A	1724	-	-	0/1/1/1	-
9	EDO	A	1721	-	-	0/1/1/1	-
9	EDO	A	1727	-	-	0/1/1/1	-
9	EDO	A	1716	-	-	0/1/1/1	-
9	EDO	B	110	-	-	0/1/1/1	-
9	EDO	A	1719	-	-	0/1/1/1	-
9	EDO	B	118	-	-	0/1/1/1	-
9	EDO	B	114	-	-	1/1/1/1	-
9	EDO	A	1725	-	-	1/1/1/1	-
9	EDO	B	113	-	-	0/1/1/1	-
9	EDO	B	119	-	-	0/1/1/1	-
9	EDO	B	115	-	-	1/1/1/1	-
9	EDO	A	1723	-	-	0/1/1/1	-
9	EDO	B	112	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	1717	-	-	0/1/1/1	-
9	EDO	C	101	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1722	EDO	O1-C1-C2-O2
9	A	1726	EDO	O1-C1-C2-O2
9	B	111	EDO	O1-C1-C2-O2
9	B	114	EDO	O1-C1-C2-O2
9	A	1725	EDO	O1-C1-C2-O2
9	B	115	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1722	EDO	1	0
9	B	116	EDO	3	0
9	B	117	EDO	2	0
9	A	1725	EDO	2	0
9	B	119	EDO	1	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 ⓘ

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	1455/1632 (89%)	0.65	165 (11%) 10 10	12, 44, 98, 147	19 (1%)
2	B	93/94 (98%)	-0.56	2 (2%) 62 66	19, 29, 59, 84	0
3	C	30/30 (100%)	0.10	0 100 100	24, 50, 74, 106	0
4	D	9/9 (100%)	0.31	0 100 100	30, 52, 94, 105	0
All	All	1587/1765 (89%)	0.56	167 (10%) 11 11	12, 43, 97, 147	19 (1%)

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1050	ILE	6.3
1	A	1066	LEU	5.8
1	A	214	PHE	5.4
1	A	1072	ILE	5.1
1	A	944	ALA	5.0
1	A	842	ILE	4.9
1	A	855	THR	4.8
1	A	123	VAL	4.8
1	A	1054	PRO	4.7
1	A	940	ILE	4.4
1	A	830	ILE	4.4
1	A	1060	PHE	4.3
1	A	1077	ILE	4.3
1	A	2	ASN	4.2
1	A	141	ASP	4.2
1	A	1143	VAL	4.1
1	A	759	TYR	4.1
1	A	856	ARG	3.9
1	A	723	LEU	3.9
1	A	1052	LEU	3.8
1	A	1185	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1302	ILE	3.8
1	A	516	TYR	3.8
1	A	902	PHE	3.7
1	A	999	GLY	3.7
1	A	1064	LEU	3.7
1	A	854	PRO	3.7
1	A	1005	LEU	3.7
1	A	730	ILE	3.6
1	A	1002	ILE	3.6
1	A	794	TYR	3.6
1	A	733	ASN	3.5
1	A	177	ILE	3.5
1	A	138	ASP	3.5
1	A	1059	ALA	3.4
1	A	258	ASP	3.4
1	A	131	PHE	3.4
1	A	428	VAL	3.4
1	A	1067	ALA	3.4
1	A	980	THR	3.4
1	A	111	TYR	3.3
1	A	431	ALA	3.3
1	A	175	THR	3.3
1	A	1190	ASN	3.3
1	A	932	ILE	3.3
1	A	147	ALA	3.3
1	A	927	ILE	3.2
1	A	298	VAL	3.2
1	A	751	GLY	3.2
1	A	112	SER	3.2
1	A	261	ILE	3.2
1	A	1065	PHE	3.2
1	A	1622	ILE	3.1
1	A	843	LEU	3.1
1	A	742	ILE	3.1
1	A	1187	ILE	3.1
1	A	1512	ILE	3.1
1	A	1071	PRO	3.1
1	A	989	CYS	3.1
1	A	1156	PRO	3.0
1	A	728	ILE	3.0
1	A	970	ILE	3.0
1	A	1076	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1078	ARG	3.0
1	A	1568	ASP	3.0
1	A	1179	ASN	3.0
1	A	291	LEU	3.0
1	A	1049	PHE	3.0
1	A	186	THR	2.9
1	A	1053	THR	2.9
1	A	1046	TYR	2.9
1	A	724	LEU	2.9
1	A	429	THR	2.9
1	A	738	CYS	2.9
1	A	981	LEU	2.8
1	A	1069	GLU	2.8
1	A	255	LEU	2.8
1	A	853	ILE	2.8
1	A	721	ARG	2.7
1	A	259	LEU	2.7
1	A	211	THR	2.7
1	A	260	ASP	2.7
1	A	743	PHE	2.7
1	A	253	THR	2.7
1	A	1594	LEU	2.7
1	A	127	LEU	2.6
1	A	134	TYR	2.6
1	A	1598	THR	2.6
1	A	146	LEU	2.6
1	A	575	GLU	2.6
1	A	916	LEU	2.5
1	A	1001	ARG	2.5
1	A	746	ILE	2.5
1	A	1000	ASN	2.5
1	A	1539	LEU	2.5
1	A	244	ALA	2.5
1	A	1063	ALA	2.5
1	A	1057	GLN	2.5
1	A	1591	LEU	2.5
1	A	295	VAL	2.5
1	A	565	GLN	2.4
1	A	144	LEU	2.4
1	A	130	ILE	2.4
1	A	720	ASN	2.4
1	A	972	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	729	ASN	2.4
1	A	911	VAL	2.4
1	A	1391	ILE	2.4
1	A	249	ARG	2.4
1	A	1	MET	2.4
1	A	987	LEU	2.4
1	A	143	TYR	2.4
1	A	747	CYS	2.3
1	A	202	LEU	2.3
1	A	973	ARG	2.3
1	A	1079	ALA	2.3
1	A	1154	ASP	2.3
1	A	126	ILE	2.3
1	A	236	ILE	2.3
1	A	1153	GLY	2.3
1	A	264	PHE	2.3
1	A	246	ILE	2.3
1	A	1207	ASP	2.3
1	A	1542	ILE	2.3
1	A	1567	ILE	2.3
1	A	150	GLN	2.2
1	A	1195	PRO	2.2
1	A	924	LEU	2.2
1	A	736	GLY	2.2
1	A	266	PHE	2.2
1	A	1191	TYR	2.2
1	A	828	ILE	2.2
1	A	988	ILE	2.2
1	A	928	SER	2.2
1	A	1074	GLN	2.2
1	A	749	ILE	2.2
1	A	1487	ILE	2.2
1	A	719	ASP	2.1
1	A	135	ASN	2.1
1	A	982	ASN	2.1
1	A	1051	ASN	2.1
1	A	1575	TYR	2.1
1	A	722	GLY	2.1
2	B	66	U	2.1
1	A	1562	LYS	2.1
1	A	187	LEU	2.1
1	A	638	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1514	LEU	2.1
1	A	1055	GLN	2.1
1	A	148	THR	2.1
1	A	1004	CYS	2.1
1	A	200	ASP	2.1
1	A	929	PRO	2.1
1	A	1062	HIS	2.1
1	A	1058	LYS	2.1
1	A	943	PHE	2.1
1	A	151	GLU	2.0
1	A	990	VAL	2.0
1	A	1566	VAL	2.0
2	B	67	U	2.0
1	A	45	LYS	2.0
1	A	1073	LYS	2.0
1	A	716	ILE	2.0
1	A	1194	TYR	2.0
1	A	1576	PHE	2.0
1	A	292	HIS	2.0
1	A	726	HIS	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 [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
9	EDO	A	1726	4/4	0.81	0.19	72,74,76,77	0
9	EDO	B	117	4/4	0.82	0.21	54,56,57,57	0
9	EDO	A	1727	4/4	0.86	0.26	76,76,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	EDO	B	116	4/4	0.86	0.17	34,43,48,49	0
9	EDO	A	1722	4/4	0.86	0.18	51,52,53,54	0
9	EDO	A	1717	4/4	0.88	0.15	35,38,39,39	0
6	NA	A	1703	1/1	0.88	0.11	64,64,64,64	0
9	EDO	B	118	4/4	0.88	0.15	44,50,52,53	0
9	EDO	B	119	4/4	0.88	0.22	57,58,58,59	0
10	ACT	B	120	4/4	0.88	0.19	57,59,60,60	0
9	EDO	A	1725	4/4	0.89	0.13	53,57,62,66	0
9	EDO	C	101	4/4	0.89	0.12	42,43,43,43	0
8	CA	A	1713	1/1	0.89	0.09	87,87,87,87	0
9	EDO	A	1724	4/4	0.93	0.10	42,42,43,43	0
8	CA	B	106	1/1	0.94	0.11	63,63,63,63	0
9	EDO	A	1716	4/4	0.94	0.11	37,41,43,44	0
9	EDO	B	114	4/4	0.94	0.12	40,43,43,46	0
8	CA	B	107	1/1	0.95	0.10	63,63,63,63	0
9	EDO	A	1721	4/4	0.95	0.09	33,34,35,35	0
8	CA	B	109	1/1	0.95	0.12	70,70,70,70	0
9	EDO	B	111	4/4	0.95	0.09	29,30,31,33	0
8	CA	A	1712	1/1	0.95	0.12	72,72,72,72	0
9	EDO	B	115	4/4	0.95	0.10	41,46,52,56	0
9	EDO	A	1723	4/4	0.96	0.10	30,35,38,42	0
8	CA	A	1710	1/1	0.96	0.12	52,52,52,52	0
8	CA	A	1714	1/1	0.96	0.09	62,62,62,62	0
8	CA	A	1711	1/1	0.96	0.06	66,66,66,66	0
9	EDO	A	1718	4/4	0.96	0.07	35,38,41,43	0
6	NA	A	1702	1/1	0.96	0.09	45,45,45,45	0
10	ACT	A	1728	4/4	0.96	0.09	33,35,35,36	0
8	CA	B	108	1/1	0.96	0.09	71,71,71,71	0
8	CA	A	1706	1/1	0.97	0.08	67,67,67,67	0
9	EDO	A	1719	4/4	0.97	0.07	34,36,37,37	0
9	EDO	A	1720	4/4	0.97	0.08	31,34,36,37	0
8	CA	B	104	1/1	0.97	0.07	68,68,68,68	0
9	EDO	B	110	4/4	0.97	0.06	28,30,32,34	0
8	CA	A	1709	1/1	0.97	0.11	42,42,42,42	0
9	EDO	B	113	4/4	0.97	0.07	27,28,28,29	0
6	NA	B	102	1/1	0.97	0.09	53,53,53,53	0
7	CL	A	1704	1/1	0.98	0.07	42,42,42,42	0
9	EDO	B	112	4/4	0.98	0.04	22,23,23,24	0
8	CA	A	1708	1/1	0.98	0.06	57,57,57,57	0
8	CA	A	1715	1/1	0.98	0.14	45,45,45,45	0
6	NA	B	101	1/1	0.99	0.04	28,28,28,28	0
8	CA	A	1707	1/1	0.99	0.08	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CA	B	105	1/1	0.99	0.05	34,34,34,34	0
7	CL	A	1705	1/1	0.99	0.08	28,28,28,28	0
8	CA	B	103	1/1	1.00	0.05	32,32,32,32	0
5	ZN	A	1701	1/1	1.00	0.02	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.