



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:26 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 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

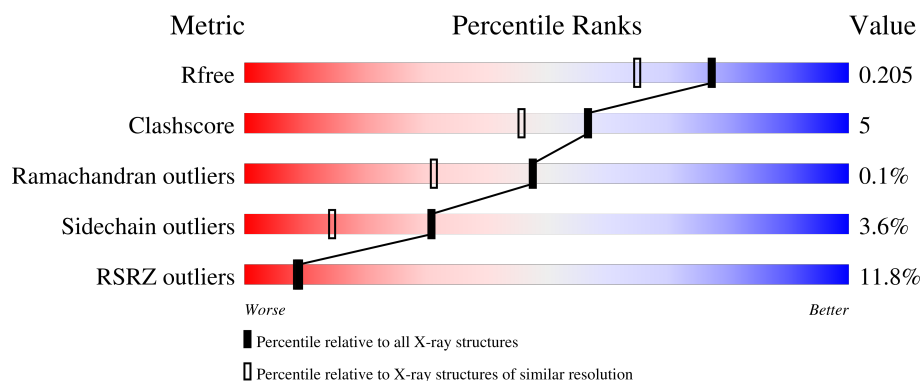
1 Overall quality at a glance

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)

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	11% 79% 9% 11%
2	B	94	% 84% 16%
3	C	30	3% 67% 33%
4	D	9	67% 33%

2 Entry composition

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
1	A	1455	Total	C	N	O	S	0	18	0
			11809	7555	2030	2193	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 DNA/RNA hybrid 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
			596	286	104	177	29			

- 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
4	D	9	Total	C	N	O	P	0	0	0
			184	89	34	53	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

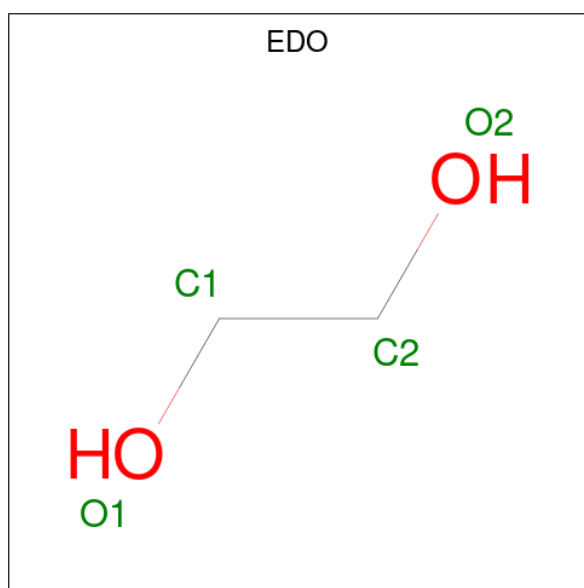
- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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	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: C₂H₆O₂).



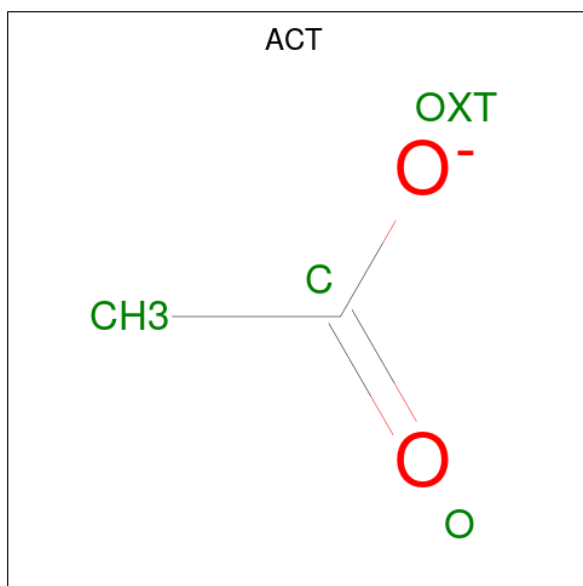
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0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

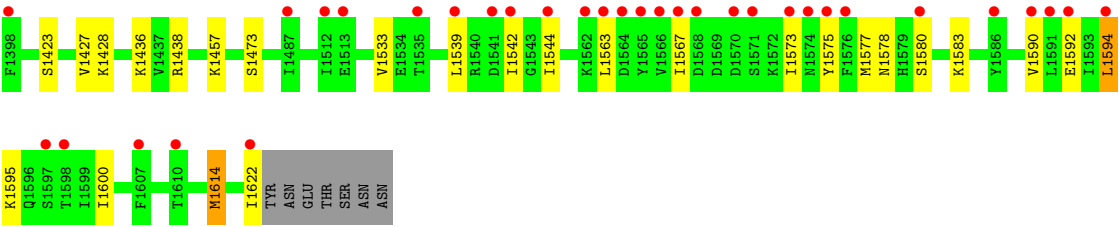
- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



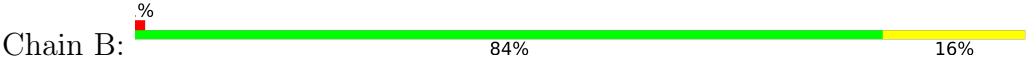
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is water.

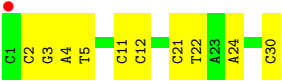
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	639	Total	O	0	0
			639	639		
11	B	342	Total	O	0	0
			342	342		
11	C	68	Total	O	0	0
			68	68		
11	D	4	Total	O	0	0
			4	4		



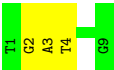
● Molecule 2: Guide RNA



● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.70Å)	Xtriage
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 ²)	28.6	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15757	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 3.18% 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: 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 ⓘ

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.

All (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
1:A:648[A]:ASP:OD2	1:A:1104:TYR:OH	2.06	0.74
1:A:1113:ASN:O	11:A:1802:HOH:O	2.09	0.70
1:A:723:LEU:HD12	1:A:727:LYS:HE3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1592:GLU:OE2	1:A:1595:LYS:NZ	2.23	0.70
3:C:22:DT:H5''	3:C:22:DT:C6	2.28	0.69
1:A:1292[B]:CYS:HB2	1:A:1332:LEU:HD21	1.77	0.67
1:A:1594:LEU:HD12	1:A:1600:ILE:HD13	1.77	0.67
11:A:2317:HOH:O	9:B:116:EDO:H12	1.96	0.66
1:A:493:TYR:O	1:A:846:LYS:NZ	2.27	0.66
3:C:2:DC:H2'	3:C:3:DG:C8	2.30	0.66
1:A:693:LEU:HG	1:A:697:LYS:HE3	1.78	0.65
1:A:54[B]:ASN:HD21	1:A:58[B]:ARG:CZ	2.10	0.65
1:A:546:LYS:HE3	3:C:30:DC:H3'	1.79	0.65
1:A:645:GLY:HA2	9:A:1722:EDO:H11	1.79	0.65
1:A:1542:ILE:HD11	1:A:1575:TYR:HD2	1.62	0.64
1:A:58[A]:ARG:NH2	11:A:1806:HOH:O	2.30	0.63
1:A:869:LEU:HD23	1:A:1095[A]:PHE:CE1	2.33	0.63
1:A:265:ASN:O	1:A:291:LEU:N	2.33	0.62
1:A:1592:GLU:HA	1:A:1595:LYS:HD3	1.82	0.61
1:A:1170:PHE:HD2	1:A:1212:ILE:HD13	1.66	0.60
3:C:4:DA:H2''	3:C:5:DT:H5''	1.84	0.60
3:C:24:DA:H5''	3:C:24:DA:H8	1.67	0.60
1:A:1236:HIS:HE1	11:A:1996:HOH:O	1.85	0.59
1:A:1573:ILE:HD12	1:A:1594:LEU:HD23	1.86	0.58
1:A:1359:GLU:OE2	11:A:1803:HOH:O	2.17	0.57
1:A:351:LYS:NZ	11:A:1814:HOH:O	2.36	0.57
2:B:66:U:H4'	2:B:67:U:O5'	2.06	0.56
1:A:982:ASN:CG	1:A:1131:ARG:HD3	2.31	0.56
1:A:419:ASP:O	1:A:423[A]:GLU:HG3	2.06	0.55
1:A:23:PHE:HB2	9:A:1726:EDO:H22	1.89	0.54
2:B:94:G:C2	9:B:118:EDO:H11	2.43	0.54
1:A:129:ASP:N	1:A:129:ASP:OD1	2.38	0.54
1:A:173:LEU:O	1:A:177:ILE:HG22	2.07	0.54
1:A:659:HIS:HD2	11:B:236:HOH:O	1.89	0.54
1:A:109:ASP:N	1:A:109:ASP:OD1	2.42	0.53
1:A:1292[A]:CYS:SG	1:A:1360:PHE:HE2	2.32	0.52
3:C:21:DC:H2'	3:C:22:DT:C6	2.44	0.52
1:A:130:ILE:HG23	1:A:134:TYR:CE2	2.45	0.51
1:A:111:TYR:O	1:A:293:HIS:HE1	1.93	0.51
1:A:1233:PHE:CZ	2:B:66:U:H5'	2.45	0.51
1:A:620:ARG:HD3	11:A:2162:HOH:O	2.09	0.51
1:A:613:LYS:HG2	11:A:2268:HOH:O	2.10	0.50
1:A:45:LYS:HB3	1:A:911:VAL:HG12	1.94	0.50
1:A:1391:ILE:HG12	1:A:1396:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:119:EDO:H12	11:B:413:HOH:O	2.11	0.50
1:A:731:ALA:HB2	1:A:739:GLU:HB3	1.94	0.50
1:A:640:LYS:HE3	2:B:68:U:C6	2.47	0.50
1:A:1436:LYS:NZ	11:A:1824:HOH:O	2.38	0.50
1:A:1577:MET:HE1	1:A:1594:LEU:HD22	1.94	0.49
1:A:159:ASN:ND2	1:A:193:TYR:OH	2.45	0.49
1:A:12:LEU:HD11	1:A:1095[B]:PHE:CE2	2.48	0.49
1:A:983:ASP:HA	1:A:1129:ASN:HD22	1.78	0.49
1:A:52:MET:HE3	1:A:864:LYS:HE2	1.95	0.49
1:A:187:LEU:O	1:A:237:GLN:NE2	2.42	0.48
1:A:52:MET:SD	9:B:116:EDO:H22	2.52	0.48
1:A:1170:PHE:CD2	1:A:1212:ILE:HD13	2.48	0.48
2:B:94:G:C6	9:B:118:EDO:H11	2.49	0.48
1:A:663[B]:GLN:HA	1:A:810:ASN:HA	1.96	0.48
1:A:10:ILE:HD13	1:A:1095[A]:PHE:HE2	1.79	0.48
1:A:130:ILE:HG22	1:A:137:GLU:OE2	2.13	0.48
1:A:514:VAL:O	1:A:529:ASP:HA	2.14	0.48
1:A:1302:ILE:H	1:A:1302:ILE:HG12	1.55	0.48
1:A:130:ILE:HG23	1:A:134:TYR:CD2	2.50	0.47
1:A:190:ILE:HG23	1:A:234:TYR:HB2	1.98	0.46
1:A:148:THR:HG22	1:A:301:ILE:HG21	1.98	0.46
1:A:1614:MET:HE3	1:A:1614:MET:HB3	1.76	0.46
2:B:66:U:H1'	2:B:67:U:OP2	2.15	0.45
1:A:664:LYS:NZ	11:A:1846:HOH:O	2.48	0.45
1:A:546:LYS:HE2	1:A:554:ASN:ND2	2.31	0.45
2:B:94:G:N1	9:B:118:EDO:H11	2.31	0.45
1:A:544[B]:ARG:NH1	1:A:549:ASP:OD1	2.50	0.45
1:A:1583:LYS:NZ	3:C:4:DA:OP1	2.50	0.45
1:A:869:LEU:HD23	1:A:1095[A]:PHE:CZ	2.52	0.44
1:A:1539:LEU:HB3	1:A:1544:ILE:HD12	1.99	0.44
1:A:4:LYS:HE2	1:A:23:PHE:CZ	2.53	0.44
1:A:266:PHE:HB2	1:A:295:VAL:CG2	2.48	0.44
1:A:111:TYR:C	1:A:293:HIS:HE1	2.26	0.44
1:A:622:ARG:HH22	3:C:30:DC:H4'	1.83	0.44
1:A:622:ARG:NH2	3:C:30:DC:H4'	2.33	0.44
1:A:1070:ASN:OD1	1:A:1072:ILE:HG12	2.17	0.44
1:A:84:ASN:OD1	11:A:1804:HOH:O	2.21	0.44
1:A:856:ARG:HH21	1:A:856:ARG:HB3	1.82	0.44
1:A:47:SER:HB3	1:A:1225:VAL:HA	2.00	0.43
1:A:1473:SER:HB3	4:D:2:DG:O4'	2.18	0.43
3:C:4:DA:C2'	3:C:5:DT:H5''	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:ALA:HA	1:A:1095[B]:PHE:CE2	2.53	0.43
1:A:894:PRO:HB3	1:A:1122:PHE:HE1	1.82	0.43
1:A:983:ASP:HA	1:A:1129:ASN:ND2	2.33	0.43
1:A:12:LEU:HD21	1:A:1095[B]:PHE:CE1	2.53	0.43
1:A:264:PHE:CE2	1:A:292:HIS:HB2	2.54	0.43
2:B:25:U:H2'	2:B:26:C:C6	2.53	0.43
1:A:640:LYS:HE2	1:A:642:ASN:HD21	1.83	0.43
1:A:1231:GLU:HG3	11:A:1830:HOH:O	2.17	0.43
1:A:1533:VAL:HB	1:A:1614:MET:HE3	1.99	0.43
1:A:54[B]:ASN:ND2	11:A:1855:HOH:O	2.51	0.43
1:A:856:ARG:HB3	1:A:856:ARG:NH2	2.34	0.43
1:A:1171:CYS:SG	1:A:1212:ILE:HD12	2.59	0.42
3:C:11:DC:H2'	3:C:12:DC:C6	2.54	0.42
1:A:550:GLU:H	1:A:550:GLU:CD	2.26	0.42
1:A:1595:LYS:HB2	1:A:1595:LYS:HE2	1.85	0.42
1:A:703:ILE:HD11	1:A:770:LEU:HD22	2.01	0.42
1:A:423[A]:GLU:CD	1:A:444:ARG:HH22	2.28	0.42
1:A:459:LYS:HG3	9:A:1722:EDO:O2	2.20	0.42
1:A:470:LEU:HB3	1:A:477:TRP:CD1	2.55	0.42
2:B:64:A:H1'	9:B:116:EDO:H21	2.02	0.42
1:A:493:TYR:CE1	1:A:544[A]:ARG:HG3	2.55	0.41
1:A:664:LYS:HA	1:A:667[B]:GLN:CG	2.50	0.41
1:A:1066:LEU:O	1:A:1073:LYS:HD2	2.19	0.41
1:A:890:GLN:HA	1:A:1116:LYS:HB3	2.02	0.41
1:A:663[B]:GLN:HG3	2:B:81:G:H5''	2.02	0.41
1:A:174:CYS:HB3	1:A:251:LEU:HB2	2.03	0.41
1:A:161:LEU:HD13	1:A:295:VAL:HB	2.03	0.41
1:A:1427:VAL:HG11	1:A:1438:ARG:HB2	2.03	0.41
1:A:54[B]:ASN:CG	1:A:58[B]:ARG:NH1	2.72	0.41
4:D:3:DA:H2''	4:D:4:DT:H72	2.03	0.41
2:B:39:A:H2'	2:B:40:G:O4'	2.21	0.41
1:A:150:GLN:OE1	1:A:152:SER:N	2.54	0.40
1:A:452:ASN:HA	2:B:89:C:N3	2.36	0.40
1:A:1047:ARG:HD2	2:B:1:G:C6	2.56	0.40
2:B:89:C:H4'	9:B:117:EDO:H22	2.04	0.40
1:A:264:PHE:CD2	1:A:292:HIS:HB2	2.57	0.40
1:A:1091:THR:O	1:A:1095[B]:PHE:HD1	2.03	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	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

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	109	ASP
1	A	127	LEU
1	A	129	ASP
1	A	133	ASP
1	A	162	MET
1	A	165	ILE
1	A	177	ILE
1	A	186	THR
1	A	187	LEU

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Mol	Chain	Res	Type
1	A	190	ILE
1	A	208	SER
1	A	210	LYS
1	A	259	LEU
1	A	295	VAL
1	A	310	ARG
1	A	343	LYS
1	A	347	ASN
1	A	351	LYS
1	A	551	LEU
1	A	592	ILE
1	A	626	LEU
1	A	716	ILE
1	A	723	LEU
1	A	725	ASN
1	A	730	ILE
1	A	791	ASN
1	A	846	LYS
1	A	987	LEU
1	A	1088	VAL
1	A	1234	ASN
1	A	1301	SER
1	A	1302	ILE
1	A	1391	ILE
1	A	1423	SER
1	A	1428	LYS
1	A	1457	LYS
1	A	1563	LEU
1	A	1567	ILE
1	A	1578	ASN
1	A	1580	SER
1	A	1590	VAL
1	A	1594	LEU
1	A	1614	MET
1	A	1622	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	293	HIS
1	A	299	ASN

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Mol	Chain	Res	Type
1	A	342	ASN
1	A	373	ASN
1	A	492	ASN
1	A	554	ASN
1	A	591	GLN
1	A	604	GLN
1	A	642	ASN
1	A	681	ASN
1	A	725	ASN
1	A	800	GLN
1	A	969	HIS
1	A	1051	ASN
1	A	1111	ASN
1	A	1129	ASN
1	A	1157	GLN
1	A	1234	ASN
1	A	1236	HIS
1	A	1504	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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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.

All (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
9	A	1717	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

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%)	0.71	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%)

All (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
1	A	2	ASN	4.6
1	A	214	PHE	4.5
1	A	721	ARG	4.4
1	A	127	LEU	4.4
1	A	999	GLY	4.4
1	A	211	THR	4.3
1	A	295	VAL	4.3
1	A	1564	ASP	4.3
1	A	1077	ILE	4.3
1	A	1060	PHE	4.2
1	A	989	CYS	4.2
1	A	723	LEU	4.1
1	A	1566	VAL	4.1
1	A	855	THR	4.1
1	A	990	VAL	4.0
1	A	1573	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	842	ILE	4.0
1	A	1594	LEU	3.9
1	A	1054	PRO	3.9
1	A	1622	ILE	3.9
1	A	1302	ILE	3.8
1	A	138	ASP	3.8
1	A	177	ILE	3.8
1	A	1575	TYR	3.8
1	A	1052	LEU	3.7
1	A	175	THR	3.7
1	A	516	TYR	3.7
1	A	856	ARG	3.7
1	A	1570	ASP	3.7
1	A	30	LEU	3.7
1	A	991	THR	3.7
1	A	141	ASP	3.6
1	A	944	ALA	3.6
1	A	111	TYR	3.6
1	A	146	LEU	3.6
1	A	1066	LEU	3.6
1	A	131	PHE	3.6
1	A	1565	TYR	3.5
1	A	728	ILE	3.5
1	A	843	LEU	3.5
1	A	1590	VAL	3.5
1	A	940	ILE	3.4
1	A	1050	ILE	3.4
1	A	980	THR	3.4
1	A	1059	ALA	3.3
1	A	112	SER	3.3
1	A	151	GLU	3.3
1	A	1541	ASP	3.3
1	A	244	ALA	3.2
1	A	246	ILE	3.2
1	A	261	ILE	3.2
1	A	1591	LEU	3.2
1	A	902	PHE	3.2
1	A	828	ILE	3.1
1	A	1002	ILE	3.1
1	A	186	THR	3.1
1	A	932	ILE	3.1
1	A	1001	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	854	PRO	3.0
1	A	1	MET	3.0
1	A	729	ASN	3.0
1	A	730	ILE	3.0
1	A	431	ALA	3.0
1	A	258	ASP	3.0
1	A	1156	PRO	3.0
1	A	1598	THR	3.0
1	A	1067	ALA	3.0
1	A	130	ILE	3.0
1	A	1185	LEU	3.0
1	A	428	VAL	2.9
1	A	147	ALA	2.9
1	A	203	ALA	2.9
1	A	33	LEU	2.9
1	A	841	ILE	2.9
1	A	1568	ASP	2.8
1	A	1143	VAL	2.8
1	A	1597	SER	2.8
1	A	1064	LEU	2.8
1	A	970	ILE	2.8
1	A	1154	ASP	2.8
1	A	726	HIS	2.8
1	A	1049	PHE	2.7
1	A	911	VAL	2.7
1	A	1214	ILE	2.7
1	A	200	ASP	2.7
1	A	134	TYR	2.7
1	A	1563	LEU	2.7
1	A	212	GLN	2.7
1	A	733	ASN	2.7
1	A	1190	ASN	2.7
1	A	1007	ASP	2.7
1	A	429	THR	2.7
1	A	1544	ILE	2.7
1	A	1069	GLU	2.6
1	A	1571	SER	2.6
1	A	943	PHE	2.6
1	A	1179	ASN	2.6
1	A	209	LEU	2.6
1	A	1539	LEU	2.6
1	A	1194	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	927	ILE	2.6
1	A	720	ASN	2.6
1	A	187	LEU	2.6
1	A	722	GLY	2.6
1	A	1083	ARG	2.6
1	A	1046	TYR	2.6
1	A	988	ILE	2.6
1	A	1181	GLY	2.5
1	A	255	LEU	2.5
1	A	298	VAL	2.5
1	A	1607	PHE	2.5
1	A	143	TYR	2.5
1	A	46	ASP	2.5
1	A	236	ILE	2.5
1	A	985	ALA	2.5
1	A	743	PHE	2.5
3	C	1	DC	2.5
1	A	190	ILE	2.5
1	A	256	THR	2.5
1	A	565	GLN	2.4
1	A	145	LYS	2.4
1	A	458	PRO	2.4
1	A	1153	GLY	2.4
1	A	125	ALA	2.4
1	A	857	ILE	2.4
1	A	1304	ILE	2.4
1	A	1390	ILE	2.4
1	A	160	LYS	2.4
1	A	1004	CYS	2.4
1	A	136	GLY	2.4
1	A	1005	LEU	2.4
1	A	1191	TYR	2.4
1	A	751	GLY	2.4
1	A	982	ASN	2.4
1	A	259	LEU	2.4
1	A	981	LEU	2.4
1	A	1398	PHE	2.4
1	A	1576	PHE	2.4
1	A	1610	THR	2.4
1	A	135	ASN	2.3
1	A	253	THR	2.3
1	A	724	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1512	ILE	2.3
1	A	168	PHE	2.3
1	A	1000	ASN	2.3
1	A	1487	ILE	2.3
1	A	639	HIS	2.2
1	A	1078	ARG	2.2
1	A	45	LYS	2.2
1	A	1065	PHE	2.2
1	A	292	HIS	2.2
1	A	1513	GLU	2.2
1	A	1187	ILE	2.2
1	A	829	LYS	2.2
1	A	1580	SER	2.2
1	A	144	LEU	2.2
1	A	1562	LYS	2.2
1	A	1586	TYR	2.2
1	A	1303	ASP	2.1
1	A	965	GLU	2.1
1	A	924	LEU	2.1
1	A	1189	LYS	2.1
1	A	1574	ASN	2.1
1	A	1182	SER	2.1
1	A	266	PHE	2.1
1	A	234	TYR	2.1
1	A	575	GLU	2.1
1	A	1055	GLN	2.1
1	A	742	ILE	2.1
1	A	794	TYR	2.1
1	A	563	LEU	2.1
1	A	967	LEU	2.1
1	A	928	SER	2.1
1	A	126	ILE	2.1
2	B	67	U	2.1
1	A	1076	VAL	2.1
1	A	738	CYS	2.1
1	A	1592	GLU	2.1
1	A	1535	THR	2.1
1	A	853	ILE	2.1
1	A	1212	ILE	2.1
1	A	1003	PHE	2.0
1	A	129	ASP	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	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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 ⓘ

There are no such residues in this entry.