



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:02 PM UTC

PDB ID : 5B2Q / pdb_00005b2q
Title : Crystal structure of Francisella novicida Cas9 RHA 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

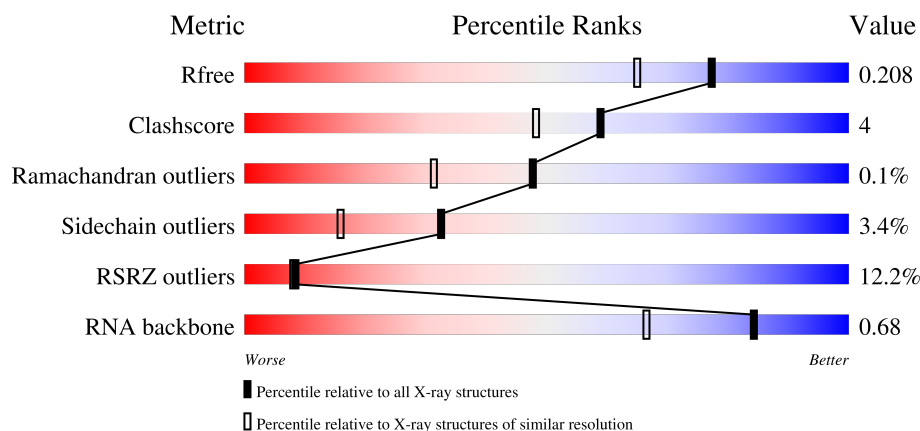
1 Overall quality at a glance

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	12% 78% 10% • 11%
2	B	94	79% 18% •
3	C	30	70% 30%
4	D	9	78% 22%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 15694 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	16	0
			11802	7550	2027	2194	31			

There are 7 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
A	1369	ARG	GLU	conflict	UNP A0Q5Y3
A	1449	HIS	GLU	conflict	UNP A0Q5Y3
A	1556	ALA	ARG	conflict	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	0	0
			1	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	10	Total	Ca	0	0
			10	10		
8	B	7	Total	Ca	0	0
			7	7		

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



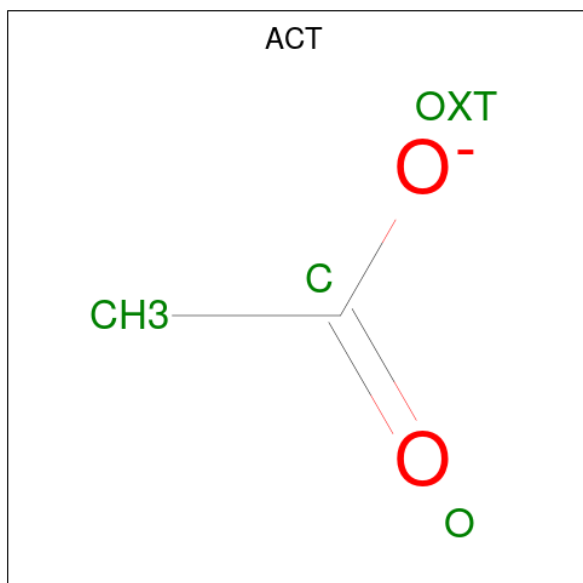
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total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

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

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

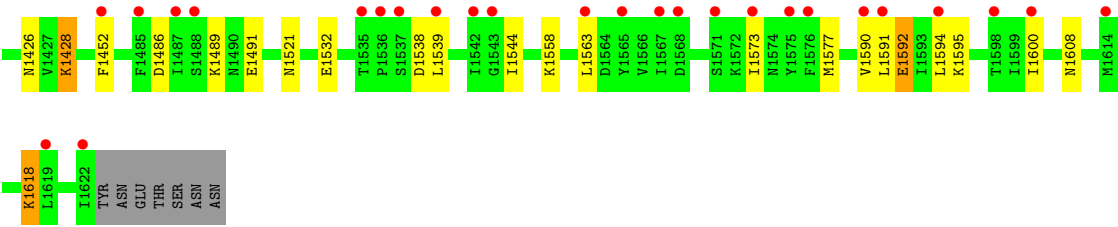
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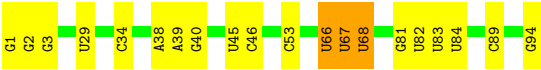
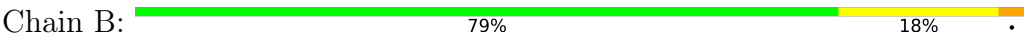
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is water.

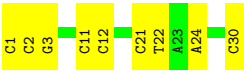
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	588	Total	O	0	0
			588	588		
11	B	334	Total	O	0	0
			334	334		
11	C	64	Total	O	0	0
			64	64		
11	D	7	Total	O	0	0
			7	7		



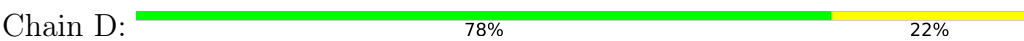
● Molecule 2: Guide RNA



● 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	81.56Å 158.98Å 96.74Å 90.00° 106.88° 90.00°	Depositor
Resolution (Å)	46.29 – 1.70 46.29 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (46.29-1.70) 98.8 (46.29-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.10_2155: ???	Depositor
R, R_{free}	0.183 , 0.206 0.185 , 0.208	Depositor DCC
R_{free} test set	12762 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15694	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: EDO, ZN, ACT, NA, CA, 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	0.34	0/12077	0.51	1/16290 (0.0%)
2	B	0.50	0/2224	0.66	0/3465
3	C	0.45	0/664	0.65	0/1018
4	D	0.37	0/207	0.61	0/319
All	All	0.37	0/15172	0.55	1/21092 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ARG	CG-CD-NE	-6.00	98.80	112.00

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	11802	0	11583	102	1
2	B	1991	0	997	13	0
3	C	595	0	337	11	0
4	D	185	0	104	1	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	0
9	B	48	0	72	3	0
10	A	8	0	6	0	0
11	A	588	0	0	9	0
11	B	334	0	0	2	0
11	C	64	0	0	1	0
11	D	7	0	0	0	0
All	All	15694	0	13171	120	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 4.

All (120) 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:265:ASN:O	1:A:291:LEU:N	2.06	0.88
1:A:906:PRO:HA	1:A:916:LEU:HD21	1.59	0.83
1:A:648[A]:ASP:OD2	1:A:1104:TYR:OH	2.03	0.76
1:A:578:LYS:NZ	1:A:582:GLU:OE2	2.20	0.75
1:A:169:LYS:HB3	1:A:187:LEU:HD11	1.68	0.74
3:C:22:DT:H5''	3:C:22:DT:H6	1.52	0.72
1:A:1486:ASP:OD1	1:A:1521:ASN:ND2	2.22	0.71
3:C:2:DC:H2'	3:C:3:DG:C8	2.25	0.70
1:A:984:GLU:O	1:A:1061:ARG:NH2	2.26	0.68
1:A:207:GLU:O	1:A:211:THR:OG1	2.13	0.66
1:A:930:GLU:O	1:A:934:LYS:NZ	2.27	0.64
1:A:645:GLY:HA2	9:A:1721:EDO:H11	1.78	0.64
1:A:23:PHE:HB2	9:A:1725:EDO:H22	1.81	0.63
1:A:1326:GLU:HG3	1:A:1327:TYR:CD2	2.34	0.62
3:C:11:DC:OP1	11:C:101:HOH:O	2.16	0.61
1:A:648[B]:ASP:OD2	1:A:1104:TYR:OH	2.19	0.60
1:A:1532:GLU:O	1:A:1618:LYS:NZ	2.31	0.60
1:A:1292[B]:CYS:HB2	1:A:1332:LEU:HD21	1.83	0.60
1:A:1302:ILE:HG22	1:A:1304:ILE:HG12	1.84	0.59
1:A:84:ASN:ND2	11:A:1803:HOH:O	2.21	0.59
1:A:622:ARG:NH2	1:A:848:GLN:OE1	2.36	0.59
1:A:1068:ASP:OD1	1:A:1068:ASP:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:GLU:OE1	1:A:785:ARG:NH2	2.25	0.58
1:A:1236:HIS:HE1	11:A:1976:HOH:O	1.85	0.58
3:C:1:DC:H6	3:C:1:DC:H5'	1.69	0.58
3:C:24:DA:H5''	3:C:24:DA:H8	1.69	0.58
1:A:1359:GLU:OE2	11:A:1801:HOH:O	2.17	0.57
1:A:174:CYS:HA	1:A:247:ASN:HD21	1.67	0.57
1:A:640:LYS:HE2	1:A:642:ASN:HD21	1.70	0.57
2:B:94:G:C2	9:B:120:EDO:H11	2.40	0.57
1:A:1577:MET:HE3	1:A:1591:LEU:HD23	1.88	0.56
4:D:7:DC:H2''	4:D:8:DG:C8	2.40	0.56
3:C:22:DT:H5''	3:C:22:DT:C6	2.38	0.55
1:A:1159:SER:OG	1:A:1221:ASP:OD1	2.17	0.55
1:A:725:ASN:HD22	1:A:794:TYR:HE2	1.54	0.55
1:A:1592:GLU:OE2	1:A:1595:LYS:NZ	2.37	0.55
1:A:169:LYS:HB3	1:A:187:LEU:CD1	2.38	0.54
1:A:159:ASN:ND2	1:A:193:TYR:OH	2.40	0.54
1:A:544[B]:ARG:NH1	1:A:549:ASP:OD1	2.41	0.53
1:A:1049:PHE:HA	1:A:1052:LEU:HD12	1.90	0.53
1:A:1539:LEU:HB3	1:A:1544:ILE:HD12	1.90	0.53
1:A:168:PHE:HA	1:A:259:LEU:HD13	1.89	0.53
1:A:1070:ASN:ND2	1:A:1072:ILE:HG12	2.24	0.52
1:A:52:MET:HE3	1:A:864:LYS:HE2	1.92	0.52
1:A:190:ILE:HG23	1:A:234:TYR:HB2	1.92	0.51
1:A:58[A]:ARG:NH2	11:A:1828:HOH:O	2.44	0.51
1:A:710:CYS:HB3	1:A:800:GLN:HB2	1.93	0.51
1:A:935:ASP:OD2	1:A:939:ARG:NH2	2.44	0.50
1:A:173:LEU:O	1:A:177:ILE:HG22	2.11	0.50
1:A:30:LEU:HD11	1:A:1212:ILE:HD11	1.93	0.50
1:A:463:LEU:HD11	1:A:853:ILE:HG12	1.93	0.50
1:A:1339:GLU:OE1	11:A:1802:HOH:O	2.20	0.50
1:A:622:ARG:HH22	3:C:30:DC:H4'	1.77	0.49
1:A:899:SER:OG	9:A:1727:EDO:H11	2.12	0.49
1:A:902:PHE:HB2	1:A:927:ILE:HG13	1.93	0.49
2:B:34:C:H6	2:B:34:C:H5''	1.77	0.49
3:C:11:DC:H2'	3:C:12:DC:C6	2.47	0.49
1:A:12:LEU:HD11	1:A:1095[B]:PHE:CE1	2.48	0.49
1:A:659:HIS:HD2	11:B:246:HOH:O	1.95	0.48
1:A:356:LEU:HB2	1:A:438:LEU:HD23	1.94	0.48
2:B:66:U:H1'	2:B:67:U:OP2	2.14	0.48
1:A:47:SER:HB3	1:A:1225:VAL:HA	1.96	0.48
2:B:45:U:H2'	2:B:46:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1240:THR:HG22	1:A:1452:PHE:HZ	1.80	0.47
1:A:37:ASN:OD1	9:A:1725:EDO:O1	2.29	0.47
1:A:549:ASP:OD1	1:A:551:LEU:HB2	2.15	0.46
1:A:169:LYS:HD3	1:A:187:LEU:HD11	1.97	0.46
1:A:622:ARG:NH2	3:C:30:DC:H4'	2.31	0.46
1:A:1070:ASN:HD22	1:A:1071:PRO:N	2.14	0.46
1:A:663[A]:GLN:HG3	2:B:81:G:H5''	1.96	0.46
1:A:869:LEU:HD23	1:A:1095[A]:PHE:CE1	2.51	0.46
1:A:426:GLN:HE21	1:A:426:GLN:HB3	1.64	0.46
1:A:640:LYS:HE3	2:B:68:U:C6	2.51	0.46
1:A:1138:GLN:O	1:A:1142:LYS:HG2	2.16	0.45
1:A:150:GLN:OE1	1:A:152:SER:N	2.49	0.45
1:A:1577:MET:HE1	1:A:1590:VAL:HG22	1.99	0.45
1:A:514:VAL:O	1:A:529:ASP:HA	2.17	0.45
9:B:119:EDO:H12	11:B:310:HOH:O	2.17	0.45
1:A:714:LEU:HG	1:A:718:LYS:HD2	1.98	0.45
3:C:21:DC:H2'	3:C:22:DT:C6	2.52	0.44
1:A:665:ARG:NH1	2:B:82:U:OP1	2.50	0.44
1:A:720:ASN:HD22	1:A:720:ASN:N	2.16	0.44
1:A:1234:ASN:HD22	1:A:1234:ASN:C	2.25	0.44
1:A:663[B]:GLN:HA	1:A:810:ASN:HA	2.00	0.44
1:A:1047:ARG:HD2	2:B:1:G:C6	2.52	0.44
1:A:1326:GLU:HG2	11:A:1893:HOH:O	2.18	0.44
1:A:1608:ASN:HB2	3:C:3:DG:OP2	2.17	0.44
1:A:1489:LYS:HG3	1:A:1491:GLU:HG2	2.00	0.44
1:A:985:ALA:HA	1:A:1061:ARG:HG2	2.00	0.44
1:A:452:ASN:HA	2:B:89:C:N3	2.33	0.43
1:A:856:ARG:HH21	1:A:856:ARG:HB3	1.84	0.43
1:A:1486:ASP:OD2	1:A:1489:LYS:HG2	2.17	0.43
1:A:1060:PHE:CE1	1:A:1076:VAL:HG22	2.54	0.43
2:B:2:G:H2'	2:B:3:G:C8	2.54	0.43
1:A:1592:GLU:HA	1:A:1595:LYS:HD3	2.00	0.43
1:A:727:LYS:HA	1:A:730:ILE:HG23	2.01	0.43
1:A:890:GLN:HA	1:A:1116:LYS:HB3	1.99	0.43
1:A:294:PHE:O	1:A:298:VAL:HG23	2.18	0.42
2:B:39:A:H2'	2:B:40:G:O4'	2.18	0.42
1:A:851:PRO:HB3	11:A:2130:HOH:O	2.19	0.42
1:A:51:LEU:HD11	1:A:912:LYS:HA	2.02	0.42
1:A:173:LEU:HD11	1:A:237:GLN:HG3	2.01	0.42
1:A:1046:TYR:CB	1:A:1079:ALA:HB1	2.50	0.42
1:A:1538:ASP:OD1	1:A:1538:ASP:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1274:LYS:O	1:A:1285:GLN:HG2	2.19	0.41
1:A:1004:CYS:HA	1:A:1065:PHE:O	2.20	0.41
1:A:1374:LYS:HE2	11:A:2002:HOH:O	2.20	0.41
2:B:38:A:H2'	2:B:39:A:C8	2.55	0.41
1:A:111:TYR:O	1:A:293:HIS:HE1	2.03	0.41
1:A:780:LYS:HE3	1:A:784:ASP:OD2	2.21	0.41
1:A:724:LEU:HD22	1:A:728:ILE:HG13	2.03	0.41
1:A:731:ALA:HB2	1:A:739:GLU:HB3	2.02	0.41
1:A:1178:ARG:NH1	1:A:1188:ASP:O	2.54	0.41
1:A:1426:ASN:O	1:A:1428:LYS:HE2	2.21	0.40
1:A:451:ASP:OD2	11:A:1804:HOH:O	2.22	0.40
1:A:982:ASN:HD21	1:A:1085:ARG:NH2	2.18	0.40
1:A:1046:TYR:HB2	1:A:1079:ALA:HB1	2.02	0.40
1:A:130:ILE:HG23	1:A:134:TYR:CE2	2.57	0.40
1:A:1563:LEU:HD11	1:A:1600:ILE:HD11	2.03	0.40
2:B:89:C:H4'	9:B:121:EDO:H11	2.04	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:NH2	1:A:1260:GLU:OE2[2_445]	2.11	0.09

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	1444/1632 (88%)	1412 (98%)	30 (2%)	2 (0%)	48 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	PHE
1	A	1128	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1260/1483 (85%)	1218 (97%)	42 (3%)	33 17

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LEU
1	A	133	ASP
1	A	137	GLU
1	A	160	LYS
1	A	165	ILE
1	A	176	ASP
1	A	177	ILE
1	A	190	ILE
1	A	208	SER
1	A	211	THR
1	A	257	ASP
1	A	259	LEU
1	A	426	GLN
1	A	435	ASP
1	A	551	LEU
1	A	626	LEU
1	A	686	LYS
1	A	720	ASN
1	A	723	LEU
1	A	724	LEU
1	A	730	ILE
1	A	828	ILE
1	A	853	ILE
1	A	939	ARG
1	A	980	THR

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Mol	Chain	Res	Type
1	A	981	LEU
1	A	982	ASN
1	A	1005	LEU
1	A	1061	ARG
1	A	1068	ASP
1	A	1077	ILE
1	A	1083	ARG
1	A	1145	SER
1	A	1176	GLU
1	A	1234	ASN
1	A	1398	PHE
1	A	1428	LYS
1	A	1558	LYS
1	A	1573	ILE
1	A	1592	GLU
1	A	1594	LEU
1	A	1618	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	247	ASN
1	A	293	HIS
1	A	299	ASN
1	A	342	ASN
1	A	426	GLN
1	A	488	GLN
1	A	492	ASN
1	A	521	GLN
1	A	599	ASN
1	A	604	GLN
1	A	617	GLN
1	A	639	HIS
1	A	642	ASN
1	A	677	GLN
1	A	720	ASN
1	A	725	ASN
1	A	800	GLN
1	A	877	ASN
1	A	938	ASN
1	A	969	HIS

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Mol	Chain	Res	Type
1	A	982	ASN
1	A	1070	ASN
1	A	1211	GLN
1	A	1234	ASN
1	A	1236	HIS
1	A	1490	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	91/94 (96%)	6 (6%)	2 (2%)

All (6) RNA backbone outliers are listed below:

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 50 ligands modelled in this entry, 24 are monoatomic - leaving 26 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	B	116	-	3,3,3	0.50	0	2,2,2	0.15	0
9	EDO	A	1722	-	3,3,3	0.48	0	2,2,2	0.28	0
9	EDO	A	1723	-	3,3,3	0.47	0	2,2,2	0.13	0
9	EDO	B	115	-	3,3,3	0.49	0	2,2,2	0.16	0
9	EDO	A	1720	-	3,3,3	0.52	0	2,2,2	0.23	0
9	EDO	B	120	-	3,3,3	0.34	0	2,2,2	0.35	0
9	EDO	A	1716	-	3,3,3	0.38	0	2,2,2	0.44	0
9	EDO	A	1719	-	3,3,3	0.59	0	2,2,2	0.32	0
9	EDO	B	119	-	3,3,3	0.46	0	2,2,2	0.04	0
10	ACT	A	1728	-	3,3,3	0.77	0	3,3,3	1.38	0
9	EDO	B	110	-	3,3,3	0.41	0	2,2,2	0.41	0
9	EDO	B	121	-	3,3,3	0.46	0	2,2,2	0.35	0
9	EDO	A	1725	-	3,3,3	0.45	0	2,2,2	0.40	0
9	EDO	B	111	-	3,3,3	0.49	0	2,2,2	0.44	0
9	EDO	A	1717	-	3,3,3	0.41	0	2,2,2	0.48	0
9	EDO	B	118	-	3,3,3	0.41	0	2,2,2	0.58	0
9	EDO	A	1721	-	3,3,3	0.34	0	2,2,2	0.56	0
9	EDO	B	113	-	3,3,3	0.64	0	2,2,2	0.11	0
9	EDO	A	1727	-	3,3,3	0.33	0	2,2,2	0.62	0
9	EDO	B	114	-	3,3,3	0.47	0	2,2,2	0.37	0
10	ACT	A	1729	-	3,3,3	0.75	0	3,3,3	1.12	0
9	EDO	B	112	-	3,3,3	0.60	0	2,2,2	0.06	0
9	EDO	A	1726	-	3,3,3	0.46	0	2,2,2	0.21	0
9	EDO	A	1718	-	3,3,3	0.46	0	2,2,2	0.06	0
9	EDO	A	1724	-	3,3,3	0.50	0	2,2,2	0.14	0
9	EDO	B	117	-	3,3,3	0.40	0	2,2,2	0.56	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	B	116	-	-	1/1/1/1	-
9	EDO	A	1722	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	1723	-	-	0/1/1/1	-
9	EDO	B	115	-	-	0/1/1/1	-
9	EDO	A	1720	-	-	0/1/1/1	-
9	EDO	B	120	-	-	0/1/1/1	-
9	EDO	A	1716	-	-	0/1/1/1	-
9	EDO	A	1719	-	-	0/1/1/1	-
9	EDO	B	119	-	-	0/1/1/1	-
9	EDO	B	110	-	-	0/1/1/1	-
9	EDO	B	121	-	-	0/1/1/1	-
9	EDO	A	1725	-	-	1/1/1/1	-
9	EDO	B	111	-	-	1/1/1/1	-
9	EDO	A	1717	-	-	0/1/1/1	-
9	EDO	B	118	-	-	1/1/1/1	-
9	EDO	A	1721	-	-	1/1/1/1	-
9	EDO	B	113	-	-	0/1/1/1	-
9	EDO	A	1727	-	-	0/1/1/1	-
9	EDO	B	114	-	-	0/1/1/1	-
9	EDO	B	112	-	-	0/1/1/1	-
9	EDO	A	1726	-	-	1/1/1/1	-
9	EDO	A	1718	-	-	0/1/1/1	-
9	EDO	A	1724	-	-	0/1/1/1	-
9	EDO	B	117	-	-	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	1726	EDO	O1-C1-C2-O2
9	A	1721	EDO	O1-C1-C2-O2
9	B	116	EDO	O1-C1-C2-O2
9	A	1725	EDO	O1-C1-C2-O2
9	B	111	EDO	O1-C1-C2-O2
9	B	118	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	120	EDO	1	0
9	B	119	EDO	1	0
9	B	121	EDO	1	0
9	A	1725	EDO	2	0
9	A	1721	EDO	1	0
9	A	1727	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%)	0.69	194 (13%) 7 6	12, 45, 101, 143	16 (1%)
2	B	93/94 (98%)	-0.56	0 100 100	19, 29, 58, 79	0
3	C	30/30 (100%)	-0.01	0 100 100	24, 51, 79, 115	0
4	D	9/9 (100%)	0.33	0 100 100	36, 52, 110, 111	0
All	All	1587/1765 (89%)	0.60	194 (12%) 8 8	12, 44, 101, 143	16 (1%)

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1060	PHE	6.3
1	A	1077	ILE	6.3
1	A	1054	PRO	5.7
1	A	1052	LEU	5.7
1	A	1059	ALA	5.6
1	A	123	VAL	5.6
1	A	1066	LEU	5.5
1	A	842	ILE	5.4
1	A	1050	ILE	5.2
1	A	855	THR	5.1
1	A	1072	ILE	4.9
1	A	999	GLY	4.9
1	A	940	ILE	4.7
1	A	2	ASN	4.6
1	A	214	PHE	4.4
1	A	843	LEU	4.3
1	A	1049	PHE	4.3
1	A	854	PRO	4.2
1	A	944	ALA	4.2
1	A	1302	ILE	4.1
1	A	759	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1064	LEU	4.0
1	A	261	ILE	3.9
1	A	980	THR	3.9
1	A	111	TYR	3.9
1	A	177	ILE	3.8
1	A	1539	LEU	3.8
1	A	112	SER	3.8
1	A	1053	THR	3.8
1	A	724	LEU	3.7
1	A	127	LEU	3.7
1	A	131	PHE	3.7
1	A	1002	ILE	3.7
1	A	429	THR	3.7
1	A	989	CYS	3.7
1	A	187	LEU	3.6
1	A	130	ILE	3.6
1	A	1063	ALA	3.6
1	A	259	LEU	3.6
1	A	733	ASN	3.6
1	A	1005	LEU	3.6
1	A	830	ILE	3.5
1	A	431	ALA	3.5
1	A	30	LEU	3.4
1	A	1067	ALA	3.4
1	A	970	ILE	3.4
1	A	295	VAL	3.4
1	A	1046	TYR	3.4
1	A	211	THR	3.4
1	A	134	TYR	3.3
1	A	151	GLU	3.3
1	A	981	LEU	3.3
1	A	1594	LEU	3.3
1	A	1591	LEU	3.3
1	A	1000	ASN	3.3
1	A	146	LEU	3.2
1	A	1065	PHE	3.2
1	A	1055	GLN	3.2
1	A	723	LEU	3.2
1	A	1568	ASP	3.2
1	A	186	THR	3.2
1	A	138	ASP	3.2
1	A	175	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	516	TYR	3.1
1	A	721	ARG	3.1
1	A	1185	LEU	3.1
1	A	253	THR	3.1
1	A	428	VAL	3.1
1	A	1057	GLN	3.1
1	A	853	ILE	3.1
1	A	932	ILE	3.1
1	A	1573	ILE	3.1
1	A	902	PHE	3.1
1	A	728	ILE	3.1
1	A	1078	ARG	3.0
1	A	856	ARG	3.0
1	A	136	GLY	3.0
1	A	141	ASP	2.9
1	A	1143	VAL	2.9
1	A	291	LEU	2.9
1	A	1542	ILE	2.9
1	A	1	MET	2.9
1	A	1076	VAL	2.9
1	A	575	GLU	2.9
1	A	1598	THR	2.9
1	A	794	TYR	2.9
1	A	973	ARG	2.9
1	A	1487	ILE	2.9
1	A	33	LEU	2.8
1	A	264	PHE	2.8
1	A	987	LEU	2.8
1	A	730	ILE	2.8
1	A	147	ALA	2.8
1	A	911	VAL	2.8
1	A	236	ILE	2.8
1	A	743	PHE	2.7
1	A	943	PHE	2.7
1	A	967	LEU	2.7
1	A	246	ILE	2.7
1	A	1190	ASN	2.7
1	A	258	ASP	2.7
1	A	1001	ARG	2.7
1	A	742	ILE	2.7
1	A	1181	GLY	2.6
1	A	1590	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	729	ASN	2.6
1	A	1058	LYS	2.6
1	A	1083	ARG	2.6
1	A	1452	PHE	2.6
1	A	738	CYS	2.6
1	A	143	TYR	2.6
1	A	1391	ILE	2.6
1	A	1045	ASN	2.6
1	A	722	GLY	2.5
1	A	1303	ASP	2.5
1	A	565	GLN	2.5
1	A	972	PRO	2.5
1	A	1195	PRO	2.5
1	A	168	PHE	2.5
1	A	747	CYS	2.5
1	A	1619	LEU	2.5
1	A	46	ASP	2.5
1	A	990	VAL	2.5
1	A	190	ILE	2.5
1	A	1075	ALA	2.5
1	A	1567	ILE	2.5
1	A	1069	GLU	2.5
1	A	1007	ASP	2.5
1	A	736	GLY	2.5
1	A	1214	ILE	2.5
1	A	1535	THR	2.5
1	A	144	LEU	2.4
1	A	1543	GLY	2.4
1	A	125	ALA	2.4
1	A	298	VAL	2.4
1	A	1622	ILE	2.4
1	A	982	ASN	2.4
1	A	1074	GLN	2.4
1	A	430	LYS	2.4
1	A	1062	HIS	2.4
1	A	266	PHE	2.4
1	A	1537	SER	2.4
1	A	751	GLY	2.4
1	A	927	ILE	2.4
1	A	1187	ILE	2.4
1	A	1156	PRO	2.3
1	A	45	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1536	PRO	2.3
1	A	1563	LEU	2.3
1	A	1485	PHE	2.3
1	A	1191	TYR	2.3
1	A	1571	SER	2.3
1	A	133	ASP	2.3
1	A	135	ASN	2.3
1	A	933	PHE	2.3
1	A	1182	SER	2.3
1	A	1576	PHE	2.3
1	A	1565	TYR	2.3
1	A	1304	ILE	2.3
1	A	1004	CYS	2.2
1	A	1600	ILE	2.2
1	A	292	HIS	2.2
1	A	984	GLU	2.2
1	A	1082	ASN	2.2
1	A	983	ASP	2.2
1	A	1614	MET	2.2
1	A	1575	TYR	2.2
1	A	986	ASN	2.2
1	A	1207	ASP	2.2
1	A	162	MET	2.1
1	A	988	ILE	2.1
1	A	1153	GLY	2.1
1	A	745	LEU	2.1
1	A	142	SER	2.1
1	A	256	THR	2.1
1	A	1209	PHE	2.1
1	A	1194	TYR	2.1
1	A	293	HIS	2.1
1	A	852	ALA	2.1
1	A	200	ASP	2.1
1	A	255	LEU	2.1
1	A	1095[A]	PHE	2.1
1	A	857	ILE	2.1
1	A	985	ALA	2.0
1	A	212	GLN	2.0
1	A	939	ARG	2.0
1	A	770	LEU	2.0
1	A	1139	LEU	2.0
1	A	148	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1056	GLU	2.0
1	A	720	ASN	2.0
1	A	165	ILE	2.0
1	A	296	PHE	2.0
1	A	1488	SER	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
6	NA	A	1703	1/1	0.81	0.14	63,63,63,63	0
9	EDO	B	119	4/4	0.82	0.22	63,65,69,70	0
9	EDO	A	1726	4/4	0.84	0.23	83,85,85,85	0
9	EDO	B	120	4/4	0.85	0.18	50,51,55,57	0
9	EDO	A	1727	4/4	0.86	0.32	81,81,82,83	0
9	EDO	B	121	4/4	0.86	0.24	56,59,61,62	0
9	EDO	B	118	4/4	0.88	0.16	45,54,58,58	0
9	EDO	A	1724	4/4	0.89	0.14	45,47,48,50	0
9	EDO	A	1725	4/4	0.90	0.11	42,45,51,57	0
9	EDO	B	117	4/4	0.90	0.16	34,46,52,55	0
10	ACT	A	1728	4/4	0.91	0.22	82,84,84,85	0
9	EDO	B	114	4/4	0.92	0.12	34,40,42,44	0
9	EDO	B	115	4/4	0.92	0.15	47,51,52,56	0
8	CA	A	1713	1/1	0.92	0.08	82,82,82,82	0
9	EDO	A	1721	4/4	0.92	0.12	45,46,47,49	0
9	EDO	A	1720	4/4	0.93	0.14	33,34,36,38	0
9	EDO	A	1723	4/4	0.94	0.11	45,45,49,52	0
9	EDO	A	1719	4/4	0.94	0.10	30,36,37,38	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	0.94	0.09	47,47,47,47	0
9	EDO	B	116	4/4	0.94	0.10	39,43,48,50	0
9	EDO	A	1716	4/4	0.94	0.12	39,45,45,47	0
8	CA	B	108	1/1	0.95	0.10	69,69,69,69	0
8	CA	B	109	1/1	0.95	0.12	70,70,70,70	0
8	CA	A	1712	1/1	0.95	0.12	72,72,72,72	0
8	CA	B	104	1/1	0.95	0.09	67,67,67,67	0
8	CA	B	107	1/1	0.95	0.10	64,64,64,64	0
9	EDO	A	1717	4/4	0.96	0.08	37,42,46,48	0
9	EDO	B	111	4/4	0.96	0.08	30,32,32,36	0
9	EDO	A	1718	4/4	0.96	0.07	32,37,38,38	0
7	CL	A	1704	1/1	0.96	0.09	43,43,43,43	0
8	CA	A	1714	1/1	0.96	0.10	69,69,69,69	0
8	CA	A	1706	1/1	0.96	0.10	67,67,67,67	0
9	EDO	A	1722	4/4	0.96	0.10	28,34,39,43	0
8	CA	A	1709	1/1	0.96	0.09	49,49,49,49	0
8	CA	A	1710	1/1	0.96	0.12	47,47,47,47	0
8	CA	A	1711	1/1	0.96	0.06	75,75,75,75	0
6	NA	B	102	1/1	0.96	0.10	59,59,59,59	0
10	ACT	A	1729	4/4	0.96	0.10	35,35,36,37	0
8	CA	B	106	1/1	0.97	0.12	44,44,44,44	0
9	EDO	B	113	4/4	0.97	0.07	29,29,31,33	0
8	CA	A	1715	1/1	0.97	0.15	54,54,54,54	0
9	EDO	B	110	4/4	0.97	0.06	31,32,35,37	0
9	EDO	B	112	4/4	0.99	0.04	23,24,24,26	0
8	CA	A	1708	1/1	0.99	0.07	47,47,47,47	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
6	NA	B	101	1/1	0.99	0.03	28,28,28,28	0
8	CA	A	1707	1/1	0.99	0.10	36,36,36,36	0
5	ZN	A	1701	1/1	1.00	0.01	25,25,25,25	0
8	CA	B	103	1/1	1.00	0.05	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.