



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:23 am BST

PDB ID : 3LOU
Title : Crystal structure of Formyltetrahydrofolate deformylase (YP_105254.1) from BURKHOLDERIA MALLEI ATCC 23344 at 1.90 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2010-02-04
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

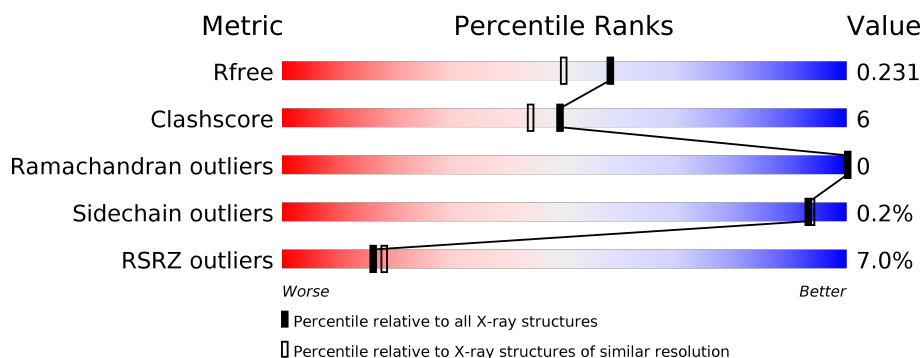
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	292	<div> <div>10%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div></div> </div> </div>
1	B	292	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div></div> </div> </div>
1	C	292	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div></div> </div> </div>
1	D	292	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div></div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UNL	A	292	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10308 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 Formyltetrahydrofolate deformylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	Se	0	14	0
			2315	1484	412	408	5	6			
1	B	279	Total	C	N	O	S	Se	0	21	0
			2335	1506	422	396	5	6			
1	C	281	Total	C	N	O	S	Se	0	13	0
			2286	1473	405	397	5	6			
1	D	279	Total	C	N	O	S	Se	0	14	0
			2296	1476	409	400	5	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP Q62DH4
B	0	GLY	-	leader sequence	UNP Q62DH4
C	0	GLY	-	leader sequence	UNP Q62DH4
D	0	GLY	-	leader sequence	UNP Q62DH4

- Molecule 2 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			5	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



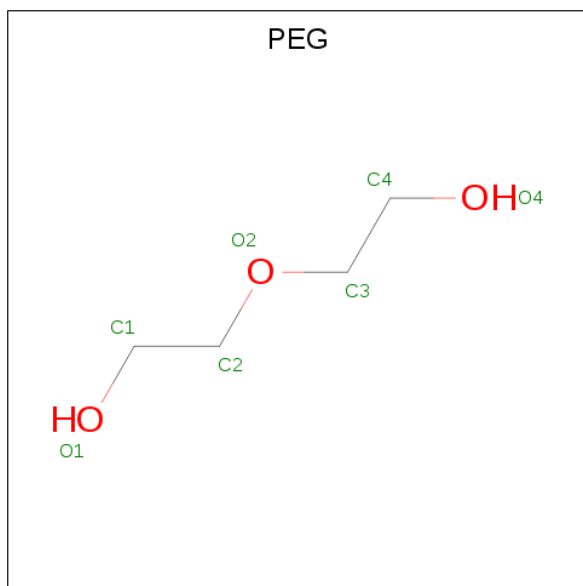
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

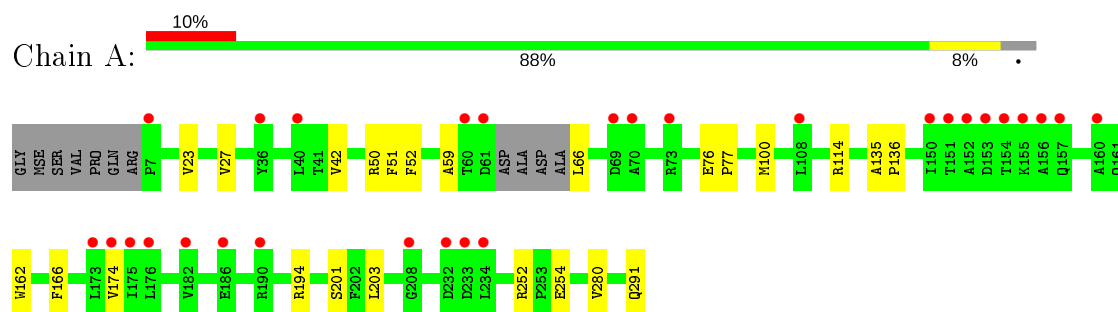
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	202	Total	O	0	1
			202	202		
6	B	226	Total	O	0	2
			227	227		
6	C	199	Total	O	0	0
			199	199		
6	D	242	Total	O	0	2
			242	242		

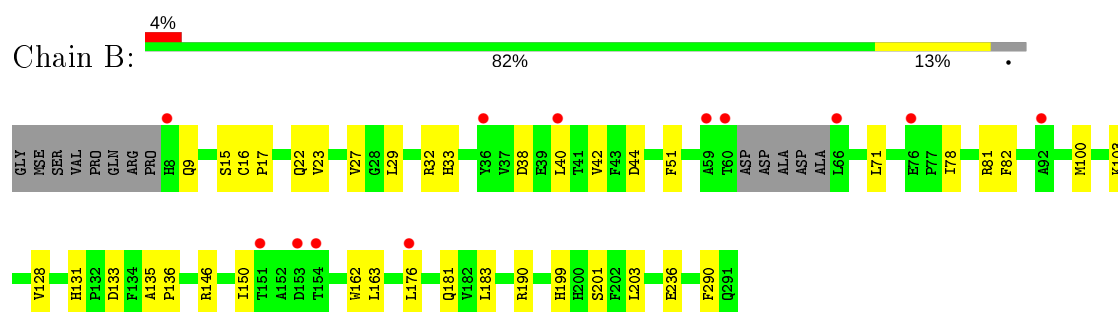
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

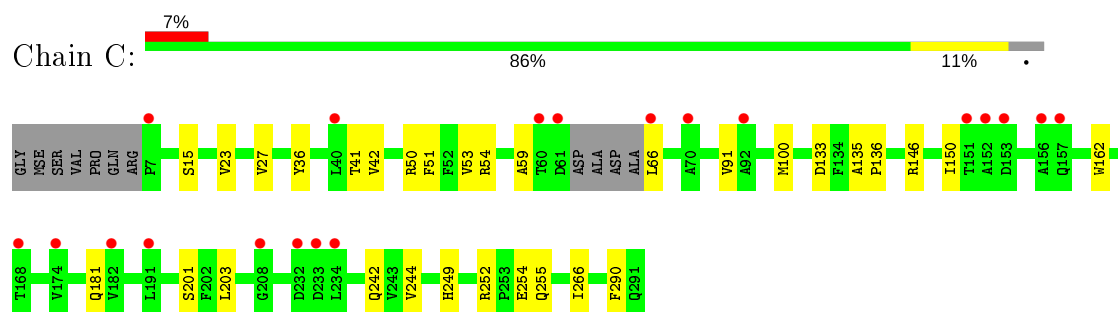
- Molecule 1: Formyltetrahydrofolate deformylase



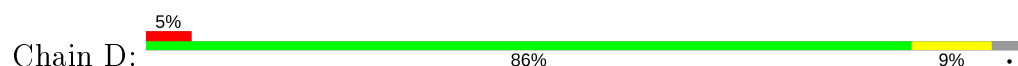
- Molecule 1: Formyltetrahydrofolate deformylase

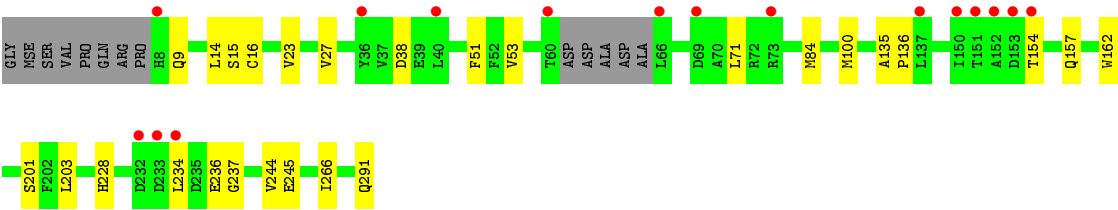


- Molecule 1: Formyltetrahydrofolate deformylase



- Molecule 1: Formyltetrahydrofolate deformylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.63Å 93.48Å 98.80Å 90.00° 95.29° 90.00°	Depositor
Resolution (Å)	29.49 – 1.90 29.49 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.49-1.90) 99.4 (29.49-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0102, PHENIX	Depositor
R, R_{free}	0.185 , 0.221 0.201 , 0.231	Depositor DCC
R_{free} test set	5276 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.6	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	0.95	EDS
Total number of atoms	10308	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.53% 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: PEG, UNL, SO4, EDO

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	0.74	0/2396	0.63	0/3241
1	B	0.75	0/2445	0.65	0/3302
1	C	0.71	0/2370	0.66	0/3207
1	D	0.75	0/2385	0.65	0/3224
All	All	0.74	0/9596	0.65	0/12974

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2315	0	2315	21	0
1	B	2335	0	2394	41	0
1	C	2286	0	2301	35	0
1	D	2296	0	2323	25	0
2	A	5	0	0	3	0
3	A	20	0	0	0	0
3	B	10	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	36	0	54	3	0
4	B	16	0	24	1	0
4	C	20	0	30	0	0
4	D	20	0	30	3	0
5	B	28	0	40	2	0
5	C	7	0	10	1	0
5	D	14	0	20	2	0
6	A	202	0	0	3	0
6	B	227	0	0	1	0
6	C	199	0	0	2	0
6	D	242	0	0	0	0
All	All	10308	0	9541	112	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 6.

All (112) 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:B:190[B]:ARG:HH11	1:B:190[B]:ARG:CG	1.63	1.12
1:B:29[B]:LEU:HD12	1:B:78:ILE:HD12	1.46	0.94
1:A:201:SER:HB3	1:B:203[B]:LEU:HD11	1.49	0.92
1:B:190[B]:ARG:HH11	1:B:190[B]:ARG:HG3	1.35	0.89
1:B:16:CYS:SG	1:B:22[A]:GLN:NE2	2.50	0.85
2:A:292:UNL:O3	2:A:292:UNL:O1	1.96	0.84
1:B:190[B]:ARG:HH11	1:B:190[B]:ARG:HG2	1.39	0.84
2:A:292:UNL:O4	2:A:292:UNL:O2	1.98	0.81
1:D:266[A]:ILE:HD12	4:D:301:EDO:H12	1.64	0.78
1:B:29[B]:LEU:HD12	1:B:78:ILE:CD1	2.14	0.76
1:C:203:LEU:HD11	1:D:201:SER:HB3	1.69	0.73
1:C:249:HIS:NE2	5:D:295:PEG:H21	2.04	0.72
1:A:252[A]:ARG:CD	1:A:254[A]:GLU:OE1	2.38	0.72
1:A:201:SER:HB3	1:B:203[B]:LEU:CD1	2.20	0.71
1:B:40:LEU:HD23	1:C:42[B]:VAL:HG21	1.73	0.69
1:B:190[B]:ARG:HG3	1:B:190[B]:ARG:NH1	2.05	0.69
1:B:29[B]:LEU:HD23	1:B:33:HIS:HD2	1.58	0.69
1:D:266[A]:ILE:HD12	4:D:301:EDO:C1	2.22	0.69
1:C:252:ARG:HG3	1:C:255:GLN:OE1	1.93	0.68
1:C:41[B]:THR:HG21	1:C:290:PHE:CD2	2.27	0.68
1:D:245[B]:GLU:OE1	4:D:301:EDO:H11	1.94	0.67
1:B:32:ARG:HD2	5:B:296:PEG:H42	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:SER:HB3	1:D:203[B]:LEU:CD1	2.27	0.65
1:C:41[B]:THR:CG2	1:C:290:PHE:CD2	2.80	0.65
1:C:41[B]:THR:HG23	1:C:290:PHE:CE2	2.32	0.64
1:A:291:GLN:HE22	1:D:291:GLN:NE2	1.96	0.64
1:B:146[A]:ARG:NH1	6:B:607:HOH:O	2.29	0.64
1:B:40:LEU:HD23	1:C:42[B]:VAL:CG2	2.26	0.64
1:C:41[B]:THR:HG22	1:C:54:ARG:HB3	1.78	0.64
2:A:292:UNL:O3	2:A:292:UNL:O2	2.18	0.62
1:C:50:ARG:HG3	6:C:364:HOH:O	2.00	0.61
1:D:100[B]:MSE:HE1	1:D:162:TRP:CD2	2.36	0.61
1:C:201:SER:HB3	1:D:203[B]:LEU:HD11	1.83	0.60
1:A:291:GLN:HE22	1:D:291:GLN:HE22	1.48	0.60
1:D:23:VAL:O	1:D:27:VAL:HG22	2.04	0.57
1:B:190[B]:ARG:NH1	1:B:190[B]:ARG:HG2	2.13	0.57
1:A:135:ALA:HB3	1:A:136:PRO:HD3	1.87	0.56
1:A:203[A]:LEU:HD11	1:B:201:SER:HB3	1.87	0.56
1:C:42[A]:VAL:HG13	1:C:51:PHE:CZ	2.41	0.55
1:A:252[A]:ARG:HD3	1:A:254[A]:GLU:OE1	2.08	0.54
1:B:29[B]:LEU:HD22	1:B:71:LEU:HG	1.90	0.54
1:B:29[B]:LEU:CD1	1:B:78:ILE:HD12	2.31	0.54
1:C:249:HIS:NE2	5:D:295:PEG:C2	2.70	0.53
1:A:59:ALA:HB2	1:A:66:LEU:HB2	1.89	0.53
1:C:244:VAL:HG21	1:D:244:VAL:HG21	1.91	0.53
1:A:194[B]:ARG:NE	6:A:307:HOH:O	2.40	0.53
1:A:23:VAL:O	1:A:27:VAL:HG22	2.09	0.53
1:D:135:ALA:HB3	1:D:136:PRO:HD3	1.90	0.53
1:A:252[A]:ARG:HD2	1:A:254[A]:GLU:OE1	2.09	0.52
4:A:303:EDO:H22	6:A:553:HOH:O	2.09	0.52
1:C:100[B]:MSE:HE1	1:C:162:TRP:CE2	2.45	0.51
1:A:201:SER:CB	1:B:203[B]:LEU:HD11	2.31	0.51
1:B:32:ARG:HD2	5:B:296:PEG:C4	2.41	0.51
1:D:15:SER:HA	1:D:51:PHE:O	2.11	0.50
1:B:163:LEU:HD22	1:B:190[B]:ARG:HD3	1.93	0.50
1:B:199:HIS:NE2	1:B:236:GLU:OE1	2.38	0.50
1:C:135:ALA:N	1:C:136:PRO:HD2	2.28	0.49
1:B:29[B]:LEU:HD23	1:B:33:HIS:CD2	2.44	0.48
1:D:236[B]:GLU:HG2	1:D:237:GLY:O	2.13	0.48
1:A:42:VAL:HG13	1:A:51:PHE:CZ	2.48	0.48
1:A:114:ARG:NH1	4:A:304:EDO:H12	2.29	0.48
1:B:290:PHE:CD1	4:B:298:EDO:H12	2.49	0.48
1:B:9:GLN:HE21	1:B:38:ASP:CG	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:VAL:O	1:B:27:VAL:HG22	2.14	0.47
1:B:176[A]:LEU:HD21	1:B:183[A]:LEU:HD11	1.97	0.47
1:C:41[B]:THR:CG2	1:C:54:ARG:HB3	2.44	0.47
1:B:135:ALA:N	1:B:136:PRO:HD2	2.31	0.46
1:D:228:HIS:CG	1:D:236[B]:GLU:HG3	2.51	0.46
1:A:100[A]:MSE:HE1	1:A:162:TRP:CE2	2.51	0.45
1:B:81[B]:ARG:HD3	1:B:82:PHE:CE2	2.51	0.45
1:A:166:PHE:CE1	1:A:174:VAL:HG23	2.51	0.45
1:B:103:LYS:HG3	1:B:131:HIS:CD2	2.51	0.45
1:C:203:LEU:CD1	1:D:201:SER:HB3	2.44	0.45
1:D:71:LEU:HD23	1:D:71:LEU:C	2.37	0.45
1:B:17:PRO:O	1:B:22[A]:GLN:NE2	2.49	0.45
1:B:150:ILE:CD1	1:B:181:GLN:HG3	2.47	0.45
1:D:100[B]:MSE:HE1	1:D:162:TRP:CE2	2.51	0.45
1:B:100[B]:MSE:HE1	1:B:162:TRP:CD2	2.52	0.44
1:B:44:ASP:OD2	1:C:36:TYR:OH	2.26	0.44
1:C:146[B]:ARG:HH11	1:C:146[B]:ARG:HA	1.83	0.44
4:A:304:EDO:C1	6:A:366:HOH:O	2.66	0.44
1:C:42[A]:VAL:CG1	1:C:51:PHE:CE1	3.01	0.44
1:C:23:VAL:O	1:C:27[B]:VAL:HG22	2.18	0.44
1:C:41[B]:THR:HG23	1:C:290:PHE:CD2	2.49	0.43
1:B:100[A]:MSE:SE	1:B:128:VAL:HB	2.69	0.43
1:C:266[B]:ILE:HD11	6:C:387:HOH:O	2.18	0.43
1:A:76:GLU:HB2	1:A:77:PRO:HD3	2.00	0.43
1:B:29[B]:LEU:CD2	1:B:71:LEU:HG	2.49	0.43
1:C:150:ILE:HD12	1:C:181:GLN:HG3	2.00	0.43
1:A:50:ARG:HG2	1:A:52:PHE:CZ	2.54	0.43
1:C:254:GLU:H	1:C:254:GLU:CD	2.21	0.43
1:C:150:ILE:CD1	1:C:181:GLN:HG3	2.49	0.42
1:C:42[A]:VAL:CG1	1:C:51:PHE:CZ	3.02	0.42
1:B:15:SER:HA	1:B:51:PHE:O	2.19	0.42
1:C:91:VAL:HG13	5:C:295:PEG:H42	2.02	0.42
1:D:9:GLN:NE2	1:D:38:ASP:OD2	2.38	0.42
1:C:135:ALA:N	1:C:136:PRO:CD	2.82	0.41
1:C:242:GLN:NE2	1:D:203[B]:LEU:HG	2.35	0.41
1:A:254[B]:GLU:CD	1:A:254[B]:GLU:H	2.24	0.41
1:C:42[B]:VAL:HG12	1:C:53:VAL:HG22	2.03	0.41
1:C:59:ALA:HB2	1:C:66:LEU:HB2	2.01	0.41
1:B:71:LEU:HD23	1:B:71:LEU:C	2.41	0.41
1:B:42[A]:VAL:CG1	1:B:51:PHE:CE1	3.04	0.41
1:D:234:LEU:HA	1:D:234:LEU:HD12	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:LEU:HG	1:D:53:VAL:HB	2.03	0.40
1:D:16:CYS:HB3	1:D:84:MSE:HG2	2.03	0.40
1:B:100[B]:MSE:HE1	1:B:162:TRP:CG	2.56	0.40
1:C:15:SER:HA	1:C:51:PHE:O	2.21	0.40
1:D:154[A]:THR:HG23	1:D:157:GLN:HB2	2.02	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	291/292 (100%)	284 (98%)	7 (2%)	0	100	100
1	B	296/292 (101%)	289 (98%)	7 (2%)	0	100	100
1	C	290/292 (99%)	284 (98%)	6 (2%)	0	100	100
1	D	289/292 (99%)	284 (98%)	5 (2%)	0	100	100
All	All	1166/1168 (100%)	1141 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	245/237 (103%)	245 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	249/237 (105%)	248 (100%)	1 (0%)	91	91
1	C	242/237 (102%)	241 (100%)	1 (0%)	91	91
1	D	245/237 (103%)	245 (100%)	0	100	100
All	All	981/948 (104%)	979 (100%)	2 (0%)	93	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	133	ASP
1	C	133	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	291	GLN
1	D	291	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 1 is unknown - leaving 42 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	$\# Z > 2$
4	EDO	A	302	-	3,3,3	0.39	0	2,2,2	0.34	0
4	EDO	D	298	-	3,3,3	0.58	0	2,2,2	0.10	0
3	SO4	B	293	-	4,4,4	0.16	0	6,6,6	0.12	0
3	SO4	C	294	-	4,4,4	0.13	0	6,6,6	0.25	0
5	PEG	C	295	-	6,6,6	0.71	0	5,5,5	0.41	0
4	EDO	A	304	-	3,3,3	0.61	0	2,2,2	0.38	0
5	PEG	B	294	-	6,6,6	0.46	0	5,5,5	0.47	0
3	SO4	A	296	-	4,4,4	0.21	0	6,6,6	0.19	0
3	SO4	D	294	-	4,4,4	0.16	0	6,6,6	0.16	0
5	PEG	B	297	-	6,6,6	0.89	0	5,5,5	0.36	0
3	SO4	A	295	-	4,4,4	0.47	0	6,6,6	0.33	0
3	SO4	D	293	-	4,4,4	0.40	0	6,6,6	0.59	0
4	EDO	D	299	-	3,3,3	0.62	0	2,2,2	0.17	0
4	EDO	B	299	-	3,3,3	0.51	0	2,2,2	0.21	0
3	SO4	A	293	-	4,4,4	0.15	0	6,6,6	0.38	0
3	SO4	B	292	-	4,4,4	0.40	0	6,6,6	0.46	0
3	SO4	A	294	-	4,4,4	0.21	0	6,6,6	0.51	0
3	SO4	D	292	-	4,4,4	0.24	0	6,6,6	0.53	0
5	PEG	B	295	-	6,6,6	0.62	0	5,5,5	0.27	0
4	EDO	B	298	-	3,3,3	0.30	0	2,2,2	0.60	0
4	EDO	C	300	-	3,3,3	0.38	0	2,2,2	0.30	0
4	EDO	D	300	-	3,3,3	0.53	0	2,2,2	0.28	0
5	PEG	B	296	-	6,6,6	0.58	0	5,5,5	0.30	0
4	EDO	C	298	-	3,3,3	0.42	0	2,2,2	0.15	0
3	SO4	C	293	-	4,4,4	0.55	0	6,6,6	0.31	0
4	EDO	C	297	-	3,3,3	0.60	0	2,2,2	0.10	0
5	PEG	D	295	-	6,6,6	0.41	0	5,5,5	0.56	0
4	EDO	D	301	-	3,3,3	0.59	0	2,2,2	0.18	0
4	EDO	A	301	-	3,3,3	0.57	0	2,2,2	0.16	0
3	SO4	C	292	-	4,4,4	0.45	0	6,6,6	0.54	0
4	EDO	A	305	-	3,3,3	0.46	0	2,2,2	0.45	0
4	EDO	C	299	-	3,3,3	0.49	0	2,2,2	0.21	0
4	EDO	C	296	-	3,3,3	0.64	0	2,2,2	0.22	0
4	EDO	A	303	-	3,3,3	0.37	0	2,2,2	0.50	0
4	EDO	B	301	-	3,3,3	0.43	0	2,2,2	0.35	0
4	EDO	A	297	-	3,3,3	0.30	0	2,2,2	0.46	0
4	EDO	B	300	-	3,3,3	0.57	0	2,2,2	0.20	0
4	EDO	A	300	-	3,3,3	0.51	0	2,2,2	0.24	0
4	EDO	D	297	-	3,3,3	0.25	0	2,2,2	0.59	0
4	EDO	A	299	-	3,3,3	0.56	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	298	-	3,3,3	0.39	0	2,2,2	0.44	0
5	PEG	D	296	-	6,6,6	0.42	0	5,5,5	0.40	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
4	EDO	A	302	-	-	1/1/1/1	-
4	EDO	D	298	-	-	1/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-
5	PEG	B	294	-	-	4/4/4/4	-
5	PEG	B	297	-	-	1/4/4/4	-
4	EDO	D	299	-	-	1/1/1/1	-
4	EDO	B	299	-	-	0/1/1/1	-
4	EDO	C	299	-	-	0/1/1/1	-
5	PEG	B	295	-	-	1/4/4/4	-
4	EDO	B	298	-	-	0/1/1/1	-
4	EDO	C	300	-	-	1/1/1/1	-
4	EDO	D	300	-	-	1/1/1/1	-
5	PEG	B	296	-	-	3/4/4/4	-
4	EDO	C	298	-	-	1/1/1/1	-
4	EDO	A	299	-	-	1/1/1/1	-
4	EDO	C	297	-	-	1/1/1/1	-
5	PEG	D	295	-	-	2/4/4/4	-
4	EDO	D	301	-	-	1/1/1/1	-
4	EDO	A	301	-	-	0/1/1/1	-
4	EDO	A	305	-	-	0/1/1/1	-
4	EDO	C	296	-	-	1/1/1/1	-
4	EDO	A	303	-	-	1/1/1/1	-
4	EDO	B	301	-	-	0/1/1/1	-
4	EDO	A	297	-	-	0/1/1/1	-
4	EDO	B	300	-	-	0/1/1/1	-
4	EDO	A	300	-	-	1/1/1/1	-
4	EDO	D	297	-	-	1/1/1/1	-
5	PEG	C	295	-	-	2/4/4/4	-
4	EDO	A	298	-	-	1/1/1/1	-
5	PEG	D	296	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	295	PEG	O2-C3-C4-O4
5	B	294	PEG	O2-C3-C4-O4
5	B	296	PEG	O1-C1-C2-O2
5	C	295	PEG	O2-C3-C4-O4
5	B	297	PEG	O1-C1-C2-O2
4	A	302	EDO	O1-C1-C2-O2
4	D	298	EDO	O1-C1-C2-O2
4	C	300	EDO	O1-C1-C2-O2
4	C	298	EDO	O1-C1-C2-O2
4	C	297	EDO	O1-C1-C2-O2
4	D	301	EDO	O1-C1-C2-O2
5	B	294	PEG	O1-C1-C2-O2
5	C	295	PEG	O1-C1-C2-O2
4	A	303	EDO	O1-C1-C2-O2
5	D	296	PEG	O1-C1-C2-O2
4	A	300	EDO	O1-C1-C2-O2
4	D	297	EDO	O1-C1-C2-O2
5	B	296	PEG	C1-C2-O2-C3
5	D	296	PEG	C4-C3-O2-C2
4	A	298	EDO	O1-C1-C2-O2
5	D	295	PEG	C4-C3-O2-C2
4	A	299	EDO	O1-C1-C2-O2
5	D	296	PEG	O2-C3-C4-O4
5	B	295	PEG	C4-C3-O2-C2
5	B	294	PEG	C4-C3-O2-C2
5	B	296	PEG	O2-C3-C4-O4
4	D	299	EDO	O1-C1-C2-O2
4	D	300	EDO	O1-C1-C2-O2
4	C	296	EDO	O1-C1-C2-O2
5	D	296	PEG	C1-C2-O2-C3
5	B	294	PEG	C1-C2-O2-C3

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	295	PEG	1	0
4	A	304	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	298	EDO	1	0
5	B	296	PEG	2	0
5	D	295	PEG	2	0
4	D	301	EDO	3	0
4	A	303	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	276/292 (94%)	0.47	29 (10%) 6 7	15, 23, 41, 51	0
1	B	274/292 (93%)	0.28	12 (4%) 34 37	15, 23, 38, 48	0
1	C	276/292 (94%)	0.46	20 (7%) 15 17	14, 23, 41, 50	0
1	D	274/292 (93%)	0.30	16 (5%) 23 25	15, 23, 37, 47	0
All	All	1100/1168 (94%)	0.38	77 (7%) 16 18	14, 23, 40, 51	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	152	ALA	7.6
1	C	153	ASP	6.4
1	A	152	ALA	6.3
1	A	234	LEU	6.1
1	C	70	ALA	6.1
1	C	233	ASP	5.7
1	B	153	ASP	5.4
1	A	153	ASP	5.4
1	C	7	PRO	5.0
1	C	234	LEU	4.9
1	C	232	ASP	4.8
1	D	60	THR	4.5
1	A	233[A]	ASP	4.5
1	C	60	THR	4.3
1	D	151	THR	4.1
1	B	8	HIS	3.9
1	D	66	LEU	3.9
1	D	152	ALA	3.9
1	A	175	ILE	3.9
1	A	151	THR	3.8
1	C	66	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	156	ALA	3.7
1	C	182[A]	VAL	3.6
1	B	60	THR	3.6
1	B	92	ALA	3.5
1	C	157	GLN	3.5
1	B	36	TYR	3.5
1	D	150	ILE	3.4
1	A	232	ASP	3.3
1	A	7	PRO	3.3
1	D	153	ASP	3.3
1	C	151	THR	3.3
1	A	174	VAL	3.2
1	C	61	ASP	3.2
1	A	156	ALA	3.2
1	D	36	TYR	3.1
1	A	154	THR	2.9
1	A	61	ASP	2.8
1	D	154[A]	THR	2.8
1	C	40	LEU	2.7
1	D	40	LEU	2.7
1	A	36	TYR	2.7
1	B	154	THR	2.7
1	B	40	LEU	2.6
1	C	208	GLY	2.6
1	A	157	GLN	2.5
1	D	233	ASP	2.5
1	A	60	THR	2.5
1	A	69[A]	ASP	2.5
1	C	92	ALA	2.4
1	A	73[A]	ARG	2.4
1	A	160	ALA	2.3
1	A	70	ALA	2.3
1	A	182	VAL	2.3
1	A	208	GLY	2.3
1	C	168	THR	2.3
1	A	150	ILE	2.2
1	A	108	LEU	2.2
1	D	69	ASP	2.2
1	B	76[A]	GLU	2.2
1	B	176[A]	LEU	2.2
1	D	137	LEU	2.2
1	B	151	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	155	LYS	2.2
1	A	40	LEU	2.2
1	B	66	LEU	2.2
1	D	234	LEU	2.2
1	C	174	VAL	2.2
1	D	232	ASP	2.1
1	A	173	LEU	2.1
1	D	73	ARG	2.1
1	B	59	ALA	2.1
1	C	191	LEU	2.1
1	A	190	ARG	2.1
1	A	176	LEU	2.1
1	D	8	HIS	2.0
1	A	186	GLU	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 carbohydrates 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(Å ²)	Q<0.9
4	EDO	D	298	4/4	0.38	0.31	74,75,75,75	0
4	EDO	D	299	4/4	0.42	0.34	61,61,62,63	0
4	EDO	D	301	4/4	0.53	0.33	68,71,71,73	0
5	PEG	B	296	7/7	0.56	0.22	64,66,72,73	0
4	EDO	B	299	4/4	0.60	0.26	57,63,63,64	0
4	EDO	D	300	4/4	0.65	0.21	50,52,55,56	0
4	EDO	A	305	4/4	0.71	0.21	58,59,60,61	0
4	EDO	B	301	4/4	0.71	0.22	62,62,62,63	0
4	EDO	C	297	4/4	0.72	0.26	49,53,53,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	299	4/4	0.74	0.24	49,51,51,52	0
5	PEG	B	297	7/7	0.76	0.21	54,56,60,60	0
4	EDO	A	301	4/4	0.76	0.28	41,53,55,59	0
4	EDO	A	298	4/4	0.76	0.24	45,47,49,50	0
5	PEG	B	295	7/7	0.77	0.21	63,65,66,66	0
4	EDO	A	300	4/4	0.77	0.20	51,54,57,60	0
4	EDO	C	296	4/4	0.77	0.17	42,47,48,51	0
4	EDO	C	300	4/4	0.79	0.28	50,51,53,56	0
5	PEG	C	295	7/7	0.80	0.27	38,53,59,61	0
4	EDO	A	304	4/4	0.80	0.18	45,50,52,56	0
4	EDO	D	297	4/4	0.81	0.17	45,45,47,51	0
4	EDO	A	302	4/4	0.82	0.28	48,53,53,55	0
5	PEG	D	296	7/7	0.82	0.27	37,50,58,63	0
4	EDO	A	303	4/4	0.84	0.18	40,40,46,47	0
5	PEG	D	295	7/7	0.84	0.18	45,47,51,51	0
4	EDO	C	299	4/4	0.85	0.19	67,67,67,67	0
4	EDO	B	298	4/4	0.86	0.23	50,52,52,52	0
5	PEG	B	294	7/7	0.86	0.27	37,51,60,67	0
3	SO4	A	296	5/5	0.87	0.23	58,60,64,71	0
4	EDO	B	300	4/4	0.87	0.15	57,58,58,60	0
4	EDO	A	297	4/4	0.88	0.11	45,50,50,52	0
2	UNL	A	292	5/-	0.88	0.13	34,39,44,48	0
3	SO4	C	294	5/5	0.91	0.20	47,53,57,61	0
4	EDO	C	298	4/4	0.92	0.18	43,44,50,51	0
3	SO4	D	292	5/5	0.94	0.14	42,48,50,56	0
3	SO4	D	294	5/5	0.95	0.18	50,51,56,57	0
3	SO4	A	293	5/5	0.96	0.13	47,48,50,56	0
3	SO4	C	293	5/5	0.96	0.18	45,49,51,52	0
3	SO4	B	293	5/5	0.97	0.15	54,57,59,60	0
3	SO4	A	294	5/5	0.97	0.14	32,39,43,43	0
3	SO4	A	295	5/5	0.97	0.15	46,49,51,53	0
3	SO4	C	292	5/5	0.97	0.12	31,40,42,43	0
3	SO4	B	292	5/5	0.98	0.11	32,32,38,39	0
3	SO4	D	293	5/5	0.98	0.12	28,28,35,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.