



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 23, 2019 – 11:18 AM EST

PDB ID : 5NX8
Title : Crystal structure of Neanderthal Adenylosuccinate Lyase (ADSL)
Authors : Van Laer, B.; Kapp, U.; Soler-Lopez, M.; Leonard, G.; Mueller-Dieckmann, C.
Deposited on : 2017-05-09
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

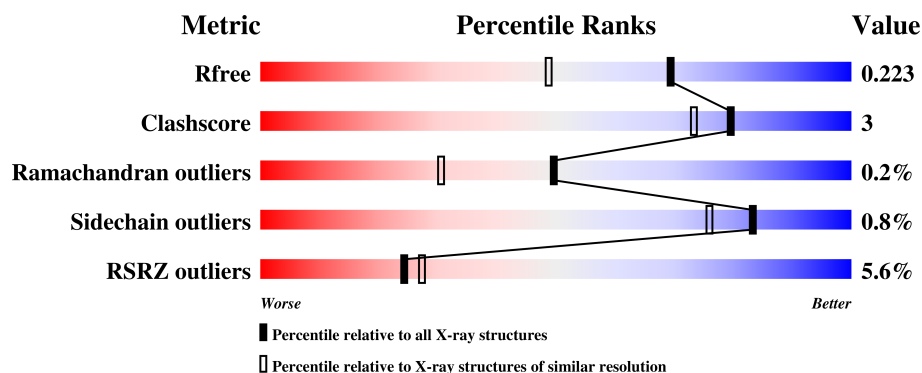
1 Overall quality at a glance ⓘ

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}	111664	3793 (1.70-1.70)
Clashscore	122126	4167 (1.70-1.70)
Ramachandran outliers	120053	4100 (1.70-1.70)
Sidechain outliers	120020	4100 (1.70-1.70)
RSRZ outliers	108989	3718 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	487	<div> <div>8%</div> <div>87% 6% 7%</div> </div>
1	B	487	<div> <div>4%</div> <div>90% 5% 5%</div> </div>
1	C	487	<div> <div>6%</div> <div>85% 7% 7%</div> </div>
1	D	487	<div> <div>3%</div> <div>90% 5% 5%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	A	502	-	-	X	-
2	PEG	C	502	-	-	X	-

2 Entry composition [i](#)

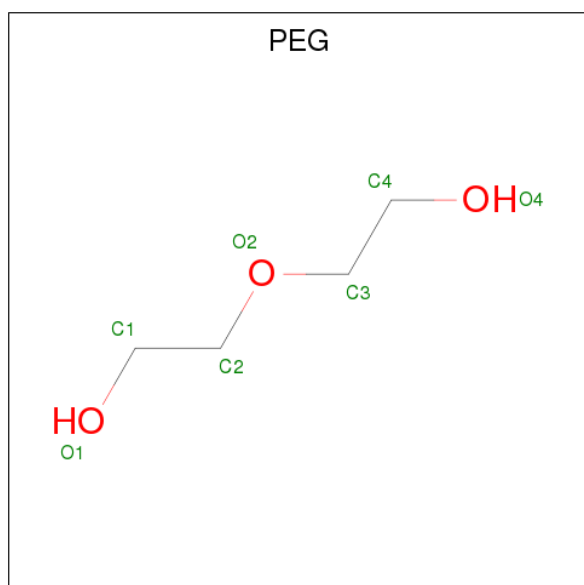
There are 5 unique types of molecules in this entry. The entry contains 16015 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenylosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	4	0
			3641	2299	641	676	25			
1	B	465	Total	C	N	O	S	0	2	0
			3727	2351	660	688	28			
1	C	451	Total	C	N	O	S	0	6	0
			3640	2290	647	677	26			
1	D	464	Total	C	N	O	S	0	4	0
			3730	2350	661	694	25			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



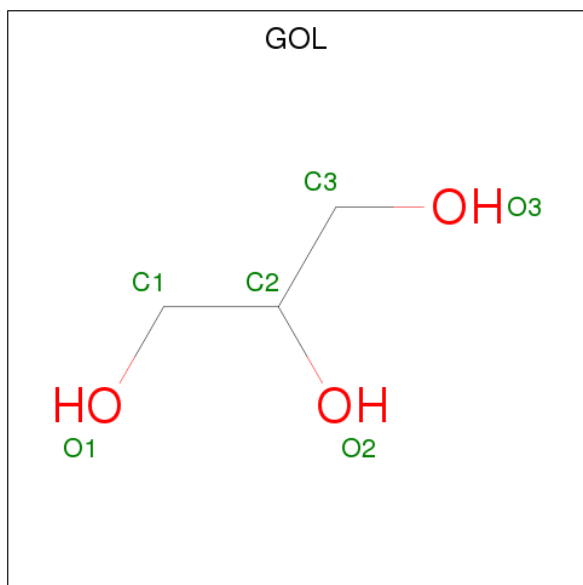
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



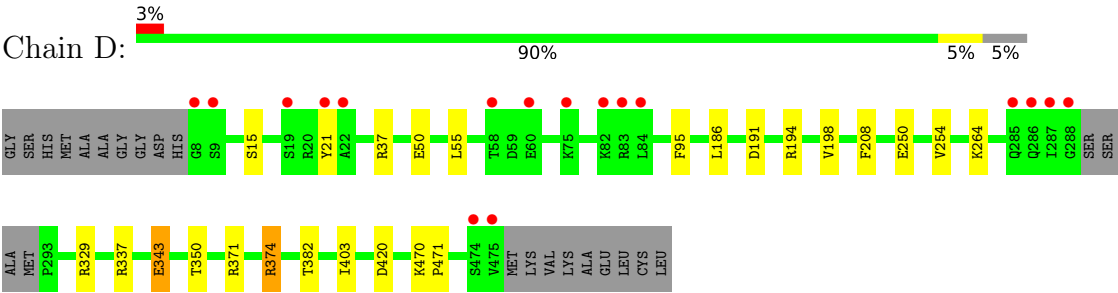
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Cl 2	0	0
4	A	2	Total 2	Cl 2	0	0
4	D	3	Total 3	Cl 3	0	0
4	C	2	Total 2	Cl 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	307	Total 307	O 307	0	0
5	B	283	Total 283	O 283	0	0
5	C	278	Total 278	O 278	0	0
5	D	323	Total 323	O 323	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.39Å 104.88Å 215.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 1.70 19.96 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.96-1.70) 99.4 (19.96-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.171 , 0.215 0.182 , 0.223	Depositor DCC
R_{free} test set	10542 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16015	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.56% 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: GOL, PEG, 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	0.76	0/3712	0.79	5/5014 (0.1%)
1	B	0.73	1/3798 (0.0%)	0.77	3/5124 (0.1%)
1	C	0.72	2/3708 (0.1%)	0.80	6/5008 (0.1%)
1	D	0.77	1/3801 (0.0%)	0.81	4/5131 (0.1%)
All	All	0.75	4/15019 (0.0%)	0.79	18/20277 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	343	GLU	CD-OE2	7.78	1.34	1.25
1	C	343	GLU	CD-OE1	6.01	1.32	1.25
1	C	280	GLU	CD-OE1	-5.63	1.19	1.25
1	D	343	GLU	CD-OE2	5.48	1.31	1.25

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	C	37	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	A	296	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	A	337	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	234	ARG	NE-CZ-NH2	-6.82	116.89	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3641	0	3658	30	0
1	B	3727	0	3758	21	0
1	C	3640	0	3654	29	0
1	D	3730	0	3745	13	0
2	A	14	0	20	8	0
2	C	14	0	20	6	0
2	D	7	0	10	0	0
3	A	12	0	16	3	0
3	B	6	0	8	0	0
3	C	12	0	16	1	0
3	D	12	0	16	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
5	A	307	0	0	9	0
5	B	283	0	0	5	0
5	C	278	0	0	5	0
5	D	323	0	0	1	0
All	All	16015	0	14921	89	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 3.

The worst 5 of 89 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:343:GLU:OE2	1:D:343:GLU:OE1	1.83	0.95
1:A:386:ILE:O	1:A:387:MET:HG2	1.68	0.94
1:A:386:ILE:O	1:A:387:MET:CG	2.16	0.93
1:A:186:LEU:HD12	1:A:254[B]:VAL:CG1	2.04	0.86
1:C:186:LEU:HD12	1:C:254[B]:VAL:CG1	2.08	0.84

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	452/487 (93%)	441 (98%)	10 (2%)	1 (0%)	49	30
1	B	463/487 (95%)	456 (98%)	6 (1%)	1 (0%)	49	30
1	C	453/487 (93%)	446 (98%)	6 (1%)	1 (0%)	49	30
1	D	464/487 (95%)	458 (99%)	5 (1%)	1 (0%)	49	30
All	All	1832/1948 (94%)	1801 (98%)	27 (2%)	4 (0%)	49	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ARG
1	B	329	ARG
1	C	329	ARG
1	D	329	ARG

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	401/422 (95%)	398 (99%)	3 (1%)	85	79
1	B	410/422 (97%)	407 (99%)	3 (1%)	85	79
1	C	401/422 (95%)	398 (99%)	3 (1%)	85	79
1	D	410/422 (97%)	406 (99%)	4 (1%)	78	69
All	All	1622/1688 (96%)	1609 (99%)	13 (1%)	83	76

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	398	ASP
1	C	190	ARG
1	D	95	PHE
1	B	264	LYS
1	D	37	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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	$\# Z > 2$
2	PEG	A	501	-	6,6,6	0.45	0	5,5,5	0.51	0
2	PEG	A	502	-	6,6,6	0.72	0	5,5,5	0.81	0
3	GOL	A	503	-	5,5,5	0.41	0	5,5,5	0.85	0
3	GOL	A	504	-	5,5,5	0.40	0	5,5,5	0.56	0
3	GOL	B	501	-	5,5,5	0.85	0	5,5,5	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEG	C	501	-	6,6,6	0.41	0	5,5,5	0.68	0
2	PEG	C	502	-	6,6,6	0.54	0	5,5,5	0.53	0
3	GOL	C	503	-	5,5,5	0.73	0	5,5,5	1.29	1 (20%)
3	GOL	C	504	-	5,5,5	0.28	0	5,5,5	0.42	0
2	PEG	D	501	-	6,6,6	0.39	0	5,5,5	0.49	0
3	GOL	D	502	-	5,5,5	0.60	0	5,5,5	1.16	0
3	GOL	D	503	-	5,5,5	0.29	0	5,5,5	0.46	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
2	PEG	A	501	-	-	0/4/4/4	0/0/0/0
2	PEG	A	502	-	-	0/4/4/4	0/0/0/0
3	GOL	A	503	-	-	0/4/4/4	0/0/0/0
3	GOL	A	504	-	-	0/4/4/4	0/0/0/0
3	GOL	B	501	-	-	0/4/4/4	0/0/0/0
2	PEG	C	501	-	-	0/4/4/4	0/0/0/0
2	PEG	C	502	-	-	0/4/4/4	0/0/0/0
3	GOL	C	503	-	-	0/4/4/4	0/0/0/0
3	GOL	C	504	-	-	0/4/4/4	0/0/0/0
2	PEG	D	501	-	-	0/4/4/4	0/0/0/0
3	GOL	D	502	-	-	0/4/4/4	0/0/0/0
3	GOL	D	503	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	GOL	C3-C2-C1	-2.40	102.37	111.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	PEG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	PEG	6	0
3	A	504	GOL	3	0
2	C	501	PEG	2	0
2	C	502	PEG	4	0
3	C	504	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	452/487 (92%)	0.08	38 (8%) 11 13	15, 25, 69, 89	0
1	B	465/487 (95%)	0.05	20 (4%) 35 40	15, 27, 54, 67	0
1	C	451/487 (92%)	0.07	28 (6%) 20 23	15, 27, 61, 90	0
1	D	464/487 (95%)	-0.05	17 (3%) 41 47	15, 26, 51, 82	0
All	All	1832/1948 (94%)	0.04	103 (5%) 24 27	15, 26, 60, 90	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	ALA	7.6
1	A	432	TYR	7.4
1	B	478	VAL	6.6
1	A	19	SER	5.5
1	A	291	ALA	5.1

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(\AA^2)	Q<0.9
2	PEG	C	501	7/7	0.74	0.26	50,52,57,67	0
2	PEG	A	502	7/7	0.79	0.26	36,41,56,64	0
2	PEG	D	501	7/7	0.82	0.27	55,58,60,63	0
2	PEG	C	502	7/7	0.83	0.27	37,46,51,59	0
3	GOL	C	504	6/6	0.84	0.19	36,46,51,59	0
2	PEG	A	501	7/7	0.84	0.35	52,58,61,63	0
3	GOL	D	502	6/6	0.87	0.14	35,40,42,57	0
3	GOL	C	503	6/6	0.88	0.11	30,35,36,38	0
3	GOL	D	503	6/6	0.90	0.16	46,51,53,60	0
3	GOL	A	504	6/6	0.90	0.16	32,47,56,58	0
3	GOL	B	501	6/6	0.92	0.08	32,34,36,36	0
3	GOL	A	503	6/6	0.95	0.10	26,29,31,32	0
4	CL	D	506	1/1	0.96	0.04	48,48,48,48	0
4	CL	D	505	1/1	0.98	0.04	35,35,35,35	0
4	CL	B	503	1/1	0.98	0.03	36,36,36,36	0
4	CL	A	505	1/1	0.99	0.03	24,24,24,24	0
4	CL	C	505	1/1	0.99	0.05	25,25,25,25	0
4	CL	D	504	1/1	0.99	0.08	27,27,27,27	0
4	CL	B	502	1/1	0.99	0.05	29,29,29,29	0
4	CL	C	506	1/1	1.00	0.05	18,18,18,18	0
4	CL	A	506	1/1	1.00	0.06	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.