



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 18, 2025 – 11:03 AM EDT

PDB ID : 9NSJ / pdb_00009nsj
Title : Finding the exit route of hydrogen peroxide from the manganese superoxide dismutase (MnSOD) active site
Authors : Dasgupta, M.; Borgstahl, G.E.O.
Deposited on : 2025-03-17
Resolution : 1.33 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 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

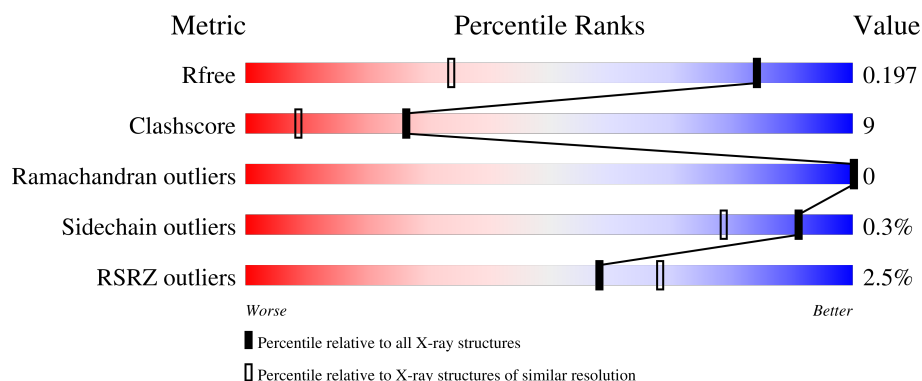
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.33 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}	164625	1904 (1.36-1.32)
Clashscore	180529	2038 (1.36-1.32)
Ramachandran outliers	177936	2016 (1.36-1.32)
Sidechain outliers	177891	2016 (1.36-1.32)
RSRZ outliers	164620	1903 (1.36-1.32)

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	199	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	B	199	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>8%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEO	A	235	-	-	X	-
2	PEO	A	257	-	-	X	-
2	PEO	A	261	-	-	X	-
2	PEO	A	265	-	-	X	-
2	PEO	B	224	-	-	X	-
2	PEO	B	232	-	-	X	-
2	PEO	B	233	-	-	X	-
2	PEO	B	249	-	-	X	-
2	PEO	B	251[A]	-	-	X	-
2	PEO	B	255	-	-	X	-
2	PEO	B	257	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8107 atoms, of which 3610 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.

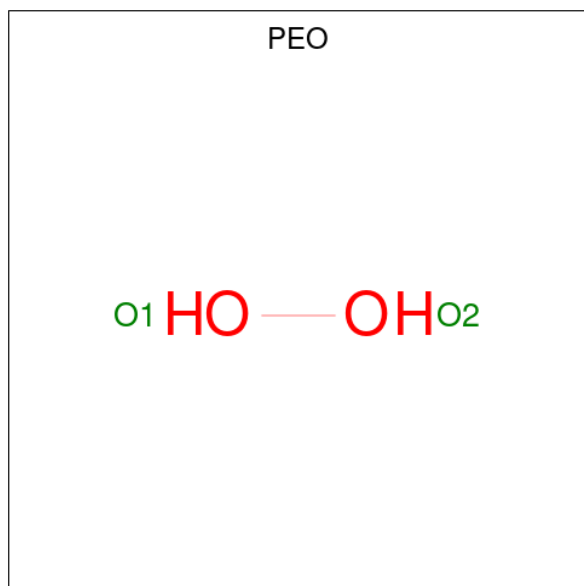
- Molecule 1 is a protein called Superoxide dismutase [Mn], mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	H	N	O	S	0	33	0
			3452	1122	1707	298	319	6			
1	B	197	Total	C	H	N	O	S	0	32	0
			3363	1091	1657	294	316	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P04179
A	143	ASN	GLN	engineered mutation	UNP P04179
B	0	MET	-	initiating methionine	UNP P04179
B	143	ASN	GLN	engineered mutation	UNP P04179

- Molecule 2 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total H O 8 4 4	0	1
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 8 4 4	0	1
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 8 4 4	0	1
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 8 4 4	0	1
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 8 4 4	0	1
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 4 2 2	0	0
2	A	1	Total H O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 8	H 4	O 4	0	1
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 8	H 4	O 4	0	1
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 8	H 4	O 4	0	1
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 8	H 4	O 4	0	1
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 8	H 4	O 4	0	1
2	A	1	Total 8	H 4	O 4	0	1

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 4	H 2	O 2	0	0
2	A	1	Total 8	H 4	O 4	0	1
2	A	1	Total 8	H 4	O 4	0	1
2	A	1	Total 4	H 2	O 2	0	0
2	B	1	Total 8	H 4	O 4	0	1
2	B	1	Total 8	H 4	O 4	0	1
2	B	1	Total 8	H 4	O 4	0	1
2	B	1	Total 4	H 2	O 2	0	0
2	B	1	Total 4	H 2	O 2	0	0
2	B	1	Total 4	H 2	O 2	0	0
2	B	1	Total 8	H 4	O 4	0	1
2	B	1	Total 4	H 2	O 2	0	0
2	B	1	Total 4	H 2	O 2	0	0
2	B	1	Total 4	H 2	O 2	0	0
2	B	1	Total 4	H 2	O 2	0	0
2	B	1	Total 4	H 2	O 2	0	0

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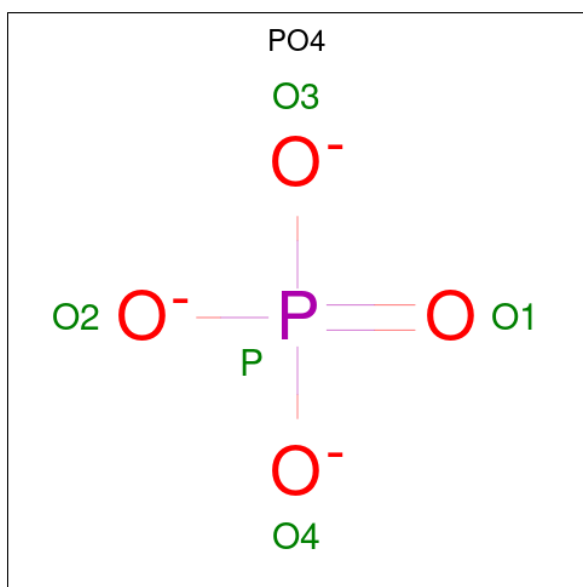
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	1
			8	4	4		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	1
			8	4	4		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	1
			8	4	4		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	0
			4	2	2		
2	B	1	Total	H	O	0	1
			8	4	4		
2	B	1	Total	H	O	0	1
			8	4	4		
2	B	1	Total	H	O	0	0
			4	2	2		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	1
			10	8	2		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	1
			10	8	2		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	K	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	6	Total K 6 6	0	0

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mn 1 1	0	0
5	B	1	Total Mn 1 1	0	0

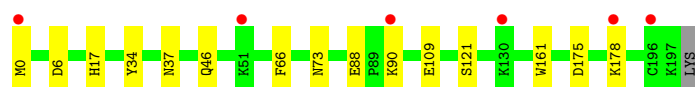
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	338	Total O 347 347	0	11
6	B	360	Total O 373 373	0	16

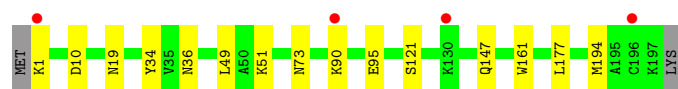
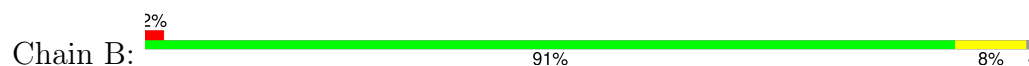
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Superoxide dismutase [Mn], mitochondrial



- Molecule 1: Superoxide dismutase [Mn], mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	78.11Å 78.11Å 236.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.34 – 1.33 39.34 – 1.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.34-1.33) 99.9 (39.34-1.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.33Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.162 , 0.196 0.163 , 0.197	Depositor DCC
R_{free} test set	2000 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	9.4	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8107	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: PO4, K, MN, PEO

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	0.58	0/1896	0.65	0/2570
1	B	0.58	0/1870	0.64	0/2542
All	All	0.58	0/3766	0.64	0/5112

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	1745	1707	1599	17	0
1	B	1706	1657	1545	14	0
2	A	132	132	0	22	0
2	B	114	114	0	25	0
3	A	30	0	0	1	0
3	B	35	0	0	0	0
4	A	7	0	0	0	0
4	B	6	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	347	0	0	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	373	0	0	13	0
All	All	4497	3610	3144	65	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 9.

The worst 5 of 65 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)
2:B:230:PEO:O1	6:B:302:HOH:O	1.79	0.99
2:A:239[A]:PEO:O1	6:A:303:HOH:O	1.81	0.95
1:A:34[A]:TYR:OH	6:A:302:HOH:O	1.85	0.94
2:B:219:PEO:O2	2:B:255:PEO:O1	1.85	0.93
1:B:1:LYS:O	6:B:304:HOH:O	1.85	0.92

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	230/199 (116%)	225 (98%)	5 (2%)	0	100	100
1	B	227/199 (114%)	223 (98%)	4 (2%)	0	100	100
All	All	457/398 (115%)	448 (98%)	9 (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	190/163 (117%)	190 (100%)	0	100	100
1	B	188/163 (115%)	187 (100%)	1 (0%)	86	69
All	All	378/326 (116%)	377 (100%)	1 (0%)	91	79

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	177	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	84	ASN
1	A	142	ASN
1	B	57	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 151 ligands modelled in this entry, 15 are monoatomic - leaving 136 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	PEO	A	259	-	1,1,1	0.24	0	-		
2	PEO	A	239[A]	-	1,1,1	0.16	0	-		
2	PEO	B	204[A]	-	1,1,1	0.31	0	-		
2	PEO	B	258[B]	-	1,1,1	0.15	0	-		
2	PEO	A	208[A]	-	1,1,1	0.27	0	-		
3	PO4	A	204	-	4,4,4	0.94	0	6,6,6	0.52	0
2	PEO	B	234	-	1,1,1	0.13	0	-		
2	PEO	A	247[B]	-	1,1,1	0.12	0	-		
2	PEO	B	245	4	1,1,1	0.09	0	-		
3	PO4	B	208	-	4,4,4	0.92	0	6,6,6	0.43	0
3	PO4	B	202[B]	4	4,4,4	1.08	0	6,6,6	0.55	0
2	PEO	A	251	-	1,1,1	0.24	0	-		
2	PEO	B	251[B]	-	1,1,1	0.01	0	-		
2	PEO	B	244	-	1,1,1	0.13	0	-		
2	PEO	B	226[A]	-	1,1,1	0.14	0	-		
2	PEO	A	264[A]	4	1,1,1	0.18	0	-		
2	PEO	A	215[A]	-	1,1,1	0.26	0	-		
2	PEO	A	248	-	1,1,1	0.15	0	-		
2	PEO	A	223[A]	-	1,1,1	0.65	0	-		
2	PEO	B	213	-	1,1,1	0.19	0	-		
2	PEO	A	201[A]	-	1,1,1	0.17	0	-		
2	PEO	B	256	-	1,1,1	0.10	0	-		
2	PEO	A	265	4	1,1,1	0.18	0	-		
2	PEO	A	246	-	1,1,1	0.16	0	-		
3	PO4	A	205[B]	-	4,4,4	0.93	0	6,6,6	0.49	0
2	PEO	B	220	-	1,1,1	0.13	0	-		
2	PEO	B	206	-	1,1,1	0.19	0	-		
2	PEO	A	216	-	1,1,1	0.15	0	-		
2	PEO	A	221[B]	-	1,1,1	0.08	0	-		
2	PEO	B	209	-	1,1,1	0.15	0	-		
2	PEO	B	228	-	1,1,1	0.22	0	-		
2	PEO	B	219	-	1,1,1	0.14	0	-		
2	PEO	B	248	-	1,1,1	0.11	0	-		
2	PEO	B	260	-	1,1,1	0.21	0	-		
2	PEO	A	263[B]	4	1,1,1	0.15	0	-		
2	PEO	A	262	-	1,1,1	0.11	0	-		
2	PEO	B	212[A]	-	1,1,1	0.19	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEO	A	250	4	1,1,1	0.10	0	-		
2	PEO	A	254[A]	-	1,1,1	0.21	0	-		
2	PEO	A	242[A]	-	1,1,1	0.09	0	-		
2	PEO	B	203[A]	-	1,1,1	0.05	0	-		
2	PEO	A	222	-	1,1,1	0.04	0	-		
3	PO4	B	205	-	4,4,4	0.99	0	6,6,6	0.50	0
2	PEO	A	224	-	1,1,1	0.17	0	-		
2	PEO	A	257	-	1,1,1	0.16	0	-		
2	PEO	A	219	-	1,1,1	0.11	0	-		
2	PEO	B	249	-	1,1,1	0.12	0	-		
2	PEO	B	257	-	1,1,1	0.16	0	-		
2	PEO	A	212	-	1,1,1	0.16	0	-		
2	PEO	A	202	-	1,1,1	0.01	0	-		
2	PEO	B	253	-	1,1,1	0.15	0	-		
2	PEO	A	241	-	1,1,1	0.20	0	-		
2	PEO	A	243	-	1,1,1	0.27	0	-		
2	PEO	B	201[A]	-	1,1,1	0.25	0	-		
2	PEO	B	229[B]	-	1,1,1	0.14	0	-		
2	PEO	B	231	-	1,1,1	0.10	0	-		
2	PEO	B	259[A]	-	1,1,1	0.38	0	-		
2	PEO	A	208[B]	-	1,1,1	0.15	0	-		
2	PEO	A	233	-	1,1,1	0.22	0	-		
2	PEO	A	237	-	1,1,1	0.14	0	-		
2	PEO	A	256	-	1,1,1	0.13	0	-		
2	PEO	A	218	-	1,1,1	0.11	0	-		
2	PEO	A	213	-	1,1,1	0.14	0	-		
2	PEO	B	218	-	1,1,1	0.12	0	-		
2	PEO	A	249[A]	-	1,1,1	0.14	0	-		
2	PEO	B	243	-	1,1,1	0.17	0	-		
2	PEO	A	261	-	1,1,1	0.09	0	-		
2	PEO	B	247	-	1,1,1	0.24	0	-		
2	PEO	B	226[B]	-	1,1,1	0.12	0	-		
2	PEO	A	264[B]	4	1,1,1	0.11	0	-		
2	PEO	A	215[B]	-	1,1,1	0.15	0	-		
2	PEO	A	236	-	1,1,1	0.22	0	-		
2	PEO	B	246	-	1,1,1	0.15	0	-		
2	PEO	A	223[B]	-	1,1,1	0.05	0	-		
2	PEO	B	258[A]	-	1,1,1	0.11	0	-		
3	PO4	A	206	-	4,4,4	0.82	0	6,6,6	1.21	0
2	PEO	A	247[A]	-	1,1,1	0.07	0	-		
2	PEO	A	201[B]	-	1,1,1	0.10	0	-		
2	PEO	A	253	4	1,1,1	0.09	0	-		
2	PEO	B	233	-	1,1,1	0.16	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEO	B	225	-	1,1,1	0.13	0	-		
2	PEO	A	209	-	1,1,1	0.11	0	-		
3	PO4	A	203	-	4,4,4	0.82	0	6,6,6	0.50	0
2	PEO	B	216	5	1,1,1	0.35	0	-		
3	PO4	B	202[A]	-	4,4,4	0.92	0	6,6,6	0.84	0
2	PEO	A	255[C]	-	1,1,1	0.13	0	-		
2	PEO	A	217	-	1,1,1	0.20	0	-		
2	PEO	B	251[A]	-	1,1,1	0.14	0	-		
2	PEO	B	230	-	1,1,1	0.17	0	-		
2	PEO	B	252	-	1,1,1	0.12	0	-		
2	PEO	B	214	-	1,1,1	0.14	0	-		
2	PEO	A	252	-	1,1,1	0.11	0	-		
2	PEO	B	250	-	1,1,1	0.12	0	-		
2	PEO	B	254	-	1,1,1	0.18	0	-		
2	PEO	B	204[C]	-	1,1,1	0.07	0	-		
3	PO4	B	207	-	4,4,4	0.80	0	6,6,6	0.83	0
3	PO4	A	205[A]	-	4,4,4	0.94	0	6,6,6	0.49	0
2	PEO	A	239[B]	4	1,1,1	0.10	0	-		
2	PEO	A	258	-	1,1,1	0.08	0	-		
2	PEO	A	234	-	1,1,1	0.13	0	-		
2	PEO	B	215	-	1,1,1	0.18	0	-		
2	PEO	B	212[B]	-	1,1,1	0.08	0	-		
2	PEO	B	221	-	1,1,1	0.07	0	-		
2	PEO	B	223	-	1,1,1	0.17	0	-		
2	PEO	B	232	-	1,1,1	0.14	0	-		
2	PEO	A	244	-	1,1,1	0.11	0	-		
2	PEO	B	227	4	1,1,1	0.29	0	-		
2	PEO	A	254[B]	-	1,1,1	0.13	0	-		
2	PEO	A	235	-	1,1,1	0.12	0	-		
2	PEO	A	242[B]	-	1,1,1	0.15	0	-		
2	PEO	B	203[B]	-	1,1,1	0.13	0	-		
2	PEO	A	221[A]	-	1,1,1	0.21	0	-		
3	PO4	B	211	-	4,4,4	0.97	0	6,6,6	0.50	0
2	PEO	A	263[A]	4	1,1,1	0.14	0	-		
2	PEO	B	255	-	1,1,1	0.08	0	-		
3	PO4	A	232	-	4,4,4	0.92	0	6,6,6	0.54	0
2	PEO	A	207	5	1,1,1	0.10	0	-		
2	PEO	A	238	-	1,1,1	0.20	0	-		
2	PEO	A	260	-	1,1,1	0.13	0	-		
2	PEO	A	210	-	1,1,1	0.11	0	-		
2	PEO	B	201[B]	-	1,1,1	0.12	0	-		
2	PEO	A	214	-	1,1,1	0.20	0	-		
2	PEO	B	210	-	1,1,1	0.23	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEO	B	242	-	1,1,1	0.19	0	-		
2	PEO	B	259[B]	-	1,1,1	0.36	0	-		
2	PEO	A	240	-	1,1,1	0.05	0	-		
2	PEO	A	220	-	1,1,1	0.12	0	-		
2	PEO	A	249[B]	-	1,1,1	0.13	0	-		
2	PEO	A	211	-	1,1,1	0.18	0	-		
3	PO4	B	241	-	4,4,4	0.86	0	6,6,6	0.52	0
2	PEO	B	222	-	1,1,1	0.21	0	-		
2	PEO	A	255[A]	-	1,1,1	0.44	0	-		
2	PEO	A	245	-	1,1,1	0.20	0	-		
2	PEO	B	224	-	1,1,1	0.17	0	-		
2	PEO	B	229[A]	-	1,1,1	0.37	0	-		
2	PEO	B	217	-	1,1,1	0.18	0	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

46 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	239[A]	PEO	1	0
2	B	258[B]	PEO	1	0
2	B	245	PEO	1	0
2	B	251[B]	PEO	1	0
2	A	264[A]	PEO	1	0
2	A	248	PEO	1	0
2	A	265	PEO	2	0
2	B	206	PEO	1	0
2	B	219	PEO	1	0
2	B	260	PEO	1	0
2	A	263[B]	PEO	1	0
2	A	250	PEO	1	0
2	B	203[A]	PEO	1	0
2	A	224	PEO	1	0
2	A	257	PEO	2	0
2	B	249	PEO	2	0
2	B	257	PEO	2	0
2	B	253	PEO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	241	PEO	1	0
2	A	256	PEO	1	0
2	A	218	PEO	1	0
2	A	213	PEO	1	0
2	B	218	PEO	1	0
2	A	261	PEO	3	0
2	B	226[B]	PEO	1	0
2	A	264[B]	PEO	1	0
3	A	206	PO4	1	0
2	A	253	PEO	1	0
2	B	233	PEO	5	0
2	B	225	PEO	1	0
2	B	216	PEO	1	0
2	B	251[A]	PEO	2	0
2	B	230	PEO	1	0
2	B	252	PEO	1	0
2	B	215	PEO	1	0
2	B	232	PEO	2	0
2	A	235	PEO	2	0
2	A	221[A]	PEO	1	0
2	A	263[A]	PEO	1	0
2	B	255	PEO	2	0
2	A	207	PEO	1	0
2	A	214	PEO	1	0
2	B	242	PEO	1	0
2	A	211	PEO	1	0
2	B	222	PEO	1	0
2	B	224	PEO	2	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	198/199 (99%)	-0.19	6 (3%)	52	63	3, 11, 29, 79	20 (10%)
1	B	197/199 (98%)	-0.25	4 (2%)	64	74	4, 11, 29, 72	17 (8%)
All	All	395/398 (99%)	-0.22	10 (2%)	58	68	3, 11, 29, 79	37 (9%)

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	LYS	3.8
1	A	0	MET	3.5
1	B	90	LYS	2.6
1	A	51[A]	LYS	2.6
1	A	90	LYS	2.6

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(\AA^2)	Q<0.9
3	PO4	B	211	5/5	0.53	0.18	45,75,96,96	5
2	PEO	A	223[B]	2/2	0.57	0.23	7,8,16,19	4
2	PEO	A	223[A]	2/2	0.57	0.23	7,9,13,16	4
3	PO4	A	205[B]	5/5	0.69	0.18	35,39,57,69	5
3	PO4	A	205[A]	5/5	0.69	0.18	26,38,48,55	5
3	PO4	A	232	5/5	0.72	0.15	37,41,58,63	5
3	PO4	B	205	5/5	0.74	0.14	42,44,85,90	0
2	PEO	A	252	2/2	0.74	0.12	50,50,60,60	4
3	PO4	A	204	5/5	0.77	0.17	21,24,62,71	5
2	PEO	A	259	2/2	0.78	0.18	14,15,17,18	4
2	PEO	B	256	2/2	0.78	0.17	19,23,36,44	4
2	PEO	A	202	2/2	0.80	0.17	32,33,39,40	0
2	PEO	A	258	2/2	0.80	0.17	16,19,25,30	4
3	PO4	A	203	5/5	0.80	0.14	25,37,54,56	5
2	PEO	B	251[B]	2/2	0.82	0.17	10,12,21,25	4
2	PEO	A	250	2/2	0.82	0.20	26,26,31,32	4
2	PEO	B	251[A]	2/2	0.82	0.17	22,26,33,40	4
3	PO4	B	241	5/5	0.82	0.17	16,24,46,67	5
2	PEO	B	203[A]	2/2	0.83	0.13	19,20,23,24	4
3	PO4	A	206	5/5	0.83	0.26	4,22,25,26	5
2	PEO	B	203[B]	2/2	0.83	0.13	20,24,24,29	4
2	PEO	A	209	2/2	0.84	0.18	18,22,24,29	4
3	PO4	B	208	5/5	0.84	0.14	23,40,58,68	5
2	PEO	A	248	2/2	0.84	0.16	25,30,31,37	4
2	PEO	B	250	2/2	0.84	0.21	20,23,25,28	4
2	PEO	B	217	2/2	0.85	0.14	17,20,25,30	4
3	PO4	B	207	5/5	0.87	0.14	22,29,46,81	5
2	PEO	B	254	2/2	0.87	0.13	20,20,24,24	4
2	PEO	B	244	2/2	0.87	0.13	21,22,26,26	4
2	PEO	A	260	2/2	0.87	0.12	16,17,19,21	4
2	PEO	A	249[A]	2/2	0.88	0.11	15,18,23,28	4
2	PEO	B	220	2/2	0.88	0.14	18,22,27,32	4
2	PEO	A	249[B]	2/2	0.88	0.11	25,30,40,48	4
2	PEO	B	245	2/2	0.88	0.18	19,23,50,61	4
2	PEO	A	210	2/2	0.88	0.15	25,30,37,44	4
2	PEO	B	247	2/2	0.89	0.13	17,20,21,25	4
2	PEO	B	258[A]	2/2	0.89	0.13	21,24,25,29	4
2	PEO	B	258[B]	2/2	0.89	0.13	17,19,21,23	4
2	PEO	B	242	2/2	0.89	0.14	15,18,18,22	4
2	PEO	A	253	2/2	0.89	0.22	11,13,36,43	4
2	PEO	B	221	2/2	0.89	0.13	15,18,29,35	4
2	PEO	B	246	2/2	0.89	0.13	22,27,35,42	4
2	PEO	B	231	2/2	0.90	0.12	15,18,30,37	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PEO	A	233	2/2	0.90	0.12	19,19,22,23	4
2	PEO	A	240	2/2	0.90	0.12	19,23,30,36	4
2	PEO	A	261	2/2	0.90	0.11	22,26,33,40	4
2	PEO	A	218	2/2	0.90	0.18	21,26,47,56	4
2	PEO	B	225	2/2	0.90	0.20	17,21,49,59	4
2	PEO	B	253	2/2	0.91	0.18	23,27,35,42	4
2	PEO	A	241	2/2	0.91	0.18	19,23,23,28	4
2	PEO	B	226[A]	2/2	0.91	0.10	19,23,26,31	4
2	PEO	B	226[B]	2/2	0.91	0.10	28,32,34,39	4
2	PEO	B	248	2/2	0.91	0.13	24,29,38,45	4
2	PEO	A	215[A]	2/2	0.91	0.10	14,16,17,19	4
2	PEO	A	219	2/2	0.91	0.11	16,19,29,35	4
2	PEO	A	215[B]	2/2	0.91	0.10	18,22,28,34	4
4	K	B	238	1/1	0.91	0.11	23,23,23,23	1
2	PEO	A	211	2/2	0.92	0.18	11,13,28,34	4
2	PEO	B	222	2/2	0.92	0.13	14,17,31,37	4
2	PEO	B	260	2/2	0.92	0.11	17,19,21,23	4
2	PEO	B	228	2/2	0.92	0.14	13,16,30,36	4
4	K	A	229	1/1	0.92	0.10	18,18,18,18	1
2	PEO	B	209	2/2	0.92	0.11	15,17,18,21	4
2	PEO	A	221[A]	2/2	0.93	0.09	14,17,21,25	4
2	PEO	B	255	2/2	0.93	0.12	14,17,28,34	4
2	PEO	A	221[B]	2/2	0.93	0.09	25,30,30,37	4
2	PEO	B	227	2/2	0.93	0.14	12,14,21,26	4
2	PEO	A	264[A]	2/2	0.93	0.10	15,18,27,33	4
2	PEO	B	259[A]	2/2	0.93	0.09	8,10,12,14	4
2	PEO	B	259[B]	2/2	0.93	0.09	7,9,11,13	4
2	PEO	B	229[A]	2/2	0.93	0.12	9,11,18,21	4
2	PEO	B	229[B]	2/2	0.93	0.12	16,18,19,22	4
2	PEO	A	264[B]	2/2	0.93	0.10	11,13,43,52	4
2	PEO	B	234	2/2	0.93	0.11	23,27,30,36	4
2	PEO	A	213	2/2	0.93	0.21	17,21,50,60	4
2	PEO	A	214	2/2	0.93	0.16	13,16,26,32	4
2	PEO	A	220	2/2	0.93	0.09	20,25,30,37	4
2	PEO	B	214	2/2	0.93	0.24	23,27,43,52	0
2	PEO	A	234	2/2	0.93	0.15	14,17,40,48	4
2	PEO	B	218	2/2	0.93	0.14	14,17,39,47	4
2	PEO	A	236	2/2	0.93	0.22	11,14,30,36	4
2	PEO	A	238	2/2	0.93	0.12	13,16,27,32	4
2	PEO	A	239[A]	2/2	0.93	0.16	10,13,33,40	4
4	K	B	237	1/1	0.93	0.09	20,20,20,20	1
2	PEO	A	239[B]	2/2	0.93	0.16	11,13,25,30	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PEO	A	208[B]	2/2	0.94	0.11	12,14,22,27	4
2	PEO	A	222	2/2	0.94	0.08	11,14,18,21	4
2	PEO	A	208[A]	2/2	0.94	0.11	9,11,24,28	4
2	PEO	B	232	2/2	0.94	0.20	20,24,31,37	4
2	PEO	A	262	2/2	0.94	0.22	16,19,54,65	4
2	PEO	A	243	2/2	0.94	0.09	13,15,18,21	4
2	PEO	B	243	2/2	0.94	0.16	11,13,22,27	4
2	PEO	A	244	2/2	0.94	0.09	19,23,23,27	4
2	PEO	A	245	2/2	0.94	0.09	17,18,21,22	4
2	PEO	A	255[A]	2/2	0.94	0.09	8,9,13,16	4
2	PEO	A	255[C]	2/2	0.94	0.09	9,11,11,14	4
2	PEO	A	246	2/2	0.94	0.10	17,21,25,31	4
2	PEO	B	249	2/2	0.94	0.16	12,15,27,33	4
2	PEO	B	201[B]	2/2	0.95	0.09	19,23,24,29	4
2	PEO	A	235	2/2	0.95	0.20	17,21,58,70	0
2	PEO	A	242[A]	2/2	0.95	0.16	16,19,30,36	4
2	PEO	A	242[B]	2/2	0.95	0.16	13,16,19,23	4
2	PEO	B	210	2/2	0.95	0.10	16,19,22,26	4
2	PEO	B	213	2/2	0.95	0.14	9,11,24,29	4
2	PEO	A	254[A]	2/2	0.95	0.18	6,7,31,37	4
2	PEO	B	252	2/2	0.95	0.19	16,19,29,35	4
2	PEO	B	215	2/2	0.95	0.14	12,14,25,31	4
2	PEO	A	254[B]	2/2	0.95	0.18	12,15,24,29	4
2	PEO	A	207	2/2	0.95	0.10	5,6,14,17	4
2	PEO	A	212	2/2	0.95	0.12	16,19,34,41	4
2	PEO	B	257	2/2	0.95	0.14	15,18,34,41	4
4	K	A	227	1/1	0.95	0.09	20,20,20,20	1
4	K	A	228	1/1	0.95	0.09	26,26,26,26	1
2	PEO	A	265	2/2	0.95	0.32	11,13,42,50	4
2	PEO	B	201[A]	2/2	0.95	0.09	12,15,17,21	4
2	PEO	B	223	2/2	0.95	0.17	16,19,40,48	4
2	PEO	B	216	2/2	0.96	0.14	8,9,20,24	4
2	PEO	A	217	2/2	0.96	0.14	14,17,28,34	4
3	PO4	B	202[A]	5/5	0.96	0.09	11,14,23,31	5
3	PO4	B	202[B]	5/5	0.96	0.09	11,12,14,17	5
2	PEO	A	247[A]	2/2	0.96	0.10	9,11,39,47	4
2	PEO	B	206	2/2	0.96	0.16	9,11,29,35	4
2	PEO	A	251	2/2	0.96	0.16	9,11,27,33	4
2	PEO	B	230	2/2	0.96	0.13	17,20,39,47	4
2	PEO	A	257	2/2	0.96	0.24	14,17,45,55	4
2	PEO	A	247[B]	2/2	0.96	0.10	24,29,32,38	4
2	PEO	B	233	2/2	0.96	0.15	11,13,33,39	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PEO	B	224	2/2	0.96	0.23	13,16,42,51	4
4	K	A	231	1/1	0.96	0.05	12,12,12,12	0
2	PEO	A	237	2/2	0.96	0.17	8,10,52,63	4
2	PEO	A	216	2/2	0.96	0.13	12,15,42,51	4
4	K	B	240	1/1	0.96	0.07	18,18,18,18	1
2	PEO	A	201[A]	2/2	0.97	0.07	17,20,20,24	4
2	PEO	A	201[B]	2/2	0.97	0.07	20,24,32,38	4
2	PEO	A	256	2/2	0.97	0.10	14,17,32,39	4
2	PEO	B	219	2/2	0.97	0.16	9,10,52,62	4
2	PEO	B	212[A]	2/2	0.97	0.06	12,13,15,16	4
2	PEO	B	212[B]	2/2	0.97	0.06	22,23,27,27	4
2	PEO	A	224	2/2	0.97	0.12	13,16,29,35	4
2	PEO	B	204[A]	2/2	0.97	0.11	9,11,22,26	4
2	PEO	B	204[C]	2/2	0.97	0.11	13,15,18,22	4
4	K	B	236	1/1	0.98	0.04	14,14,14,14	1
2	PEO	A	263[A]	2/2	0.98	0.16	5,6,29,34	4
4	K	A	225	1/1	0.98	0.04	14,14,14,14	1
2	PEO	A	263[B]	2/2	0.98	0.16	7,8,8,10	4
4	K	A	226	1/1	0.99	0.03	14,14,14,14	1
4	K	B	235	1/1	0.99	0.04	13,13,13,13	1
4	K	B	239	1/1	0.99	0.05	12,12,12,12	1
4	K	A	230	1/1	0.99	0.04	14,14,14,14	1
5	MN	A	266	1/1	1.00	0.01	7,7,7,7	1
5	MN	B	261	1/1	1.00	0.02	7,7,7,7	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.