



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:15 AM UTC

PDB ID : 8X3W / pdb_00008x3w
Title : Crystal structure of DIMIT1 from the thermophilic archaeon, *Pyrococcus horikoshii*
Authors : Sayan, S.; Mandal, S.K.; Dutta, A.; Kanaujia, S.P.
Deposited on : 2023-11-14
Resolution : 2.01 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

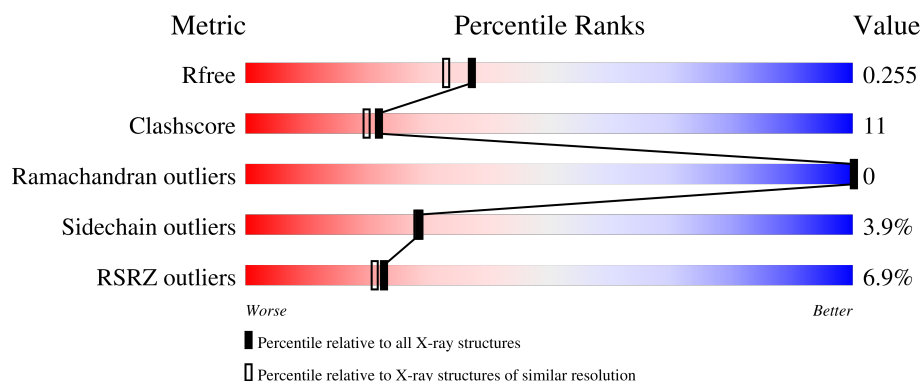
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	290	7% 76% 15% • 7%
1	B	290	6% 77% 15% • 7%

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
3	SO3	A	307	-	-	X	-
3	SO3	A	308	-	-	X	-
3	SO3	A	310	-	-	X	-
3	SO3	A	311	-	-	X	-
3	SO3	A	312	-	-	X	-
3	SO3	B	304	-	-	X	-
3	SO3	B	305	-	-	X	-
4	GOL	B	307	-	-	X	-
8	ARG	A	322	-	-	X	-
8	ARG	B	313	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4899 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 Probable ribosomal RNA small subunit methyltransferase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2195	1419	383	387	6			
1	B	270	Total	C	N	O	S	0	1	0
			2200	1422	383	389	6			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O59487
A	2	SER	-	expression tag	UNP O59487
A	3	SER	-	expression tag	UNP O59487
A	4	ARG	-	expression tag	UNP O59487
A	5	ILE	-	expression tag	UNP O59487
A	6	ARG	-	expression tag	UNP O59487
A	7	ILE	-	expression tag	UNP O59487
A	8	ASN	-	expression tag	UNP O59487
A	9	THR	-	expression tag	UNP O59487
A	10	LYS	-	expression tag	UNP O59487
A	11	SER	-	expression tag	UNP O59487
A	12	LEU	-	expression tag	UNP O59487
A	13	LEU	-	expression tag	UNP O59487
A	14	VAL	-	expression tag	UNP O59487
A	15	GLN	-	expression tag	UNP O59487
A	16	PRO	-	expression tag	UNP O59487
A	17	GLY	-	expression tag	UNP O59487
A	18	TYR	-	expression tag	UNP O59487
A	19	SER	-	expression tag	UNP O59487
A	20	GLY	-	expression tag	UNP O59487
A	21	SER	-	expression tag	UNP O59487
A	22	LYS	-	expression tag	UNP O59487
B	1	MET	-	initiating methionine	UNP O59487
B	2	SER	-	expression tag	UNP O59487
B	3	SER	-	expression tag	UNP O59487

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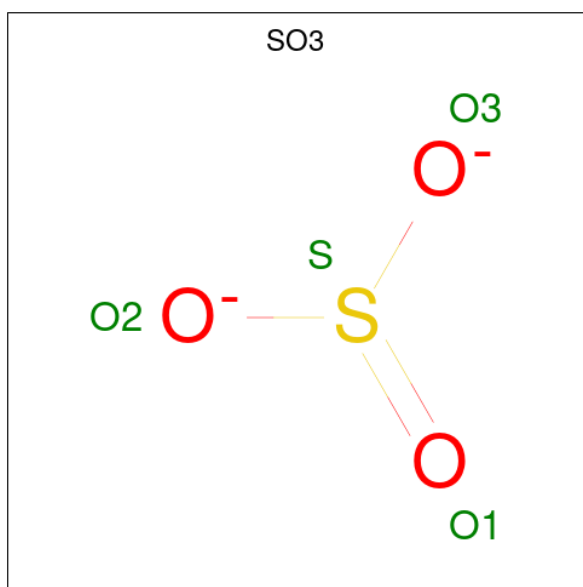
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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	ARG	-	expression tag	UNP O59487
B	5	ILE	-	expression tag	UNP O59487
B	6	ARG	-	expression tag	UNP O59487
B	7	ILE	-	expression tag	UNP O59487
B	8	ASN	-	expression tag	UNP O59487
B	9	THR	-	expression tag	UNP O59487
B	10	LYS	-	expression tag	UNP O59487
B	11	SER	-	expression tag	UNP O59487
B	12	LEU	-	expression tag	UNP O59487
B	13	LEU	-	expression tag	UNP O59487
B	14	VAL	-	expression tag	UNP O59487
B	15	GLN	-	expression tag	UNP O59487
B	16	PRO	-	expression tag	UNP O59487
B	17	GLY	-	expression tag	UNP O59487
B	18	TYR	-	expression tag	UNP O59487
B	19	SER	-	expression tag	UNP O59487
B	20	GLY	-	expression tag	UNP O59487
B	21	SER	-	expression tag	UNP O59487
B	22	LYS	-	expression tag	UNP O59487

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total 6	Zn 6	0	0
2	B	3	Total 3	Zn 3	0	0

- Molecule 3 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



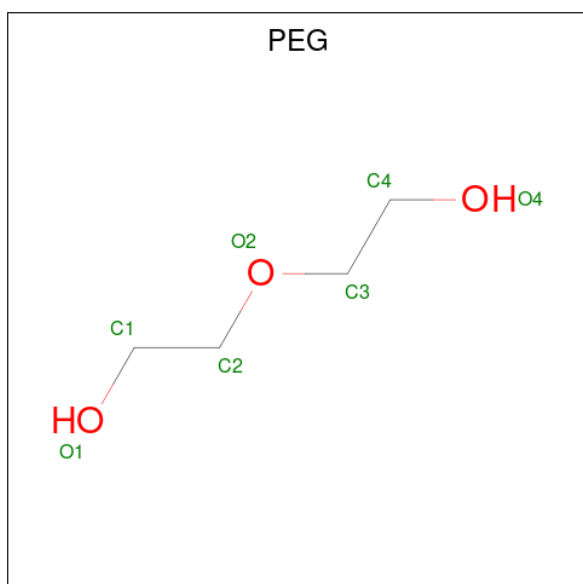
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			4	3	1		
3	A	1	Total	O	S	0	0
			4	3	1		
3	A	1	Total	O	S	0	0
			4	3	1		
3	A	1	Total	O	S	0	0
			4	3	1		
3	A	1	Total	O	S	0	0
			4	3	1		
3	B	1	Total	O	S	0	0
			4	3	1		
3	B	1	Total	O	S	0	0
			4	3	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



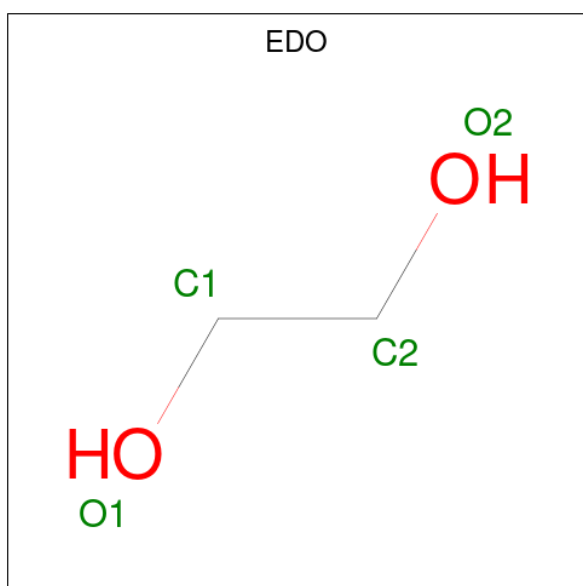
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



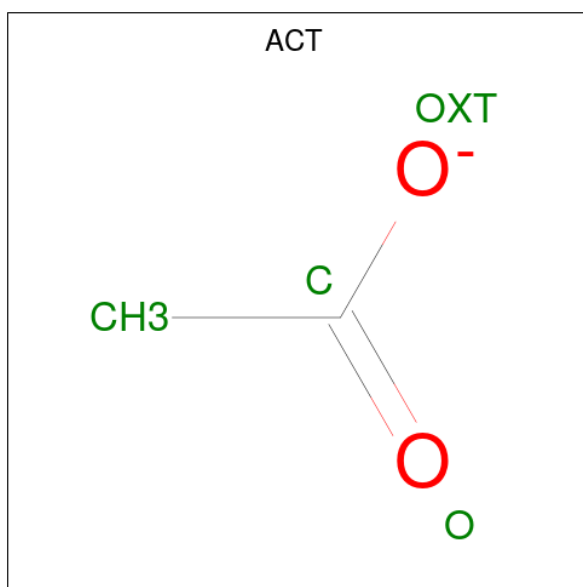
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



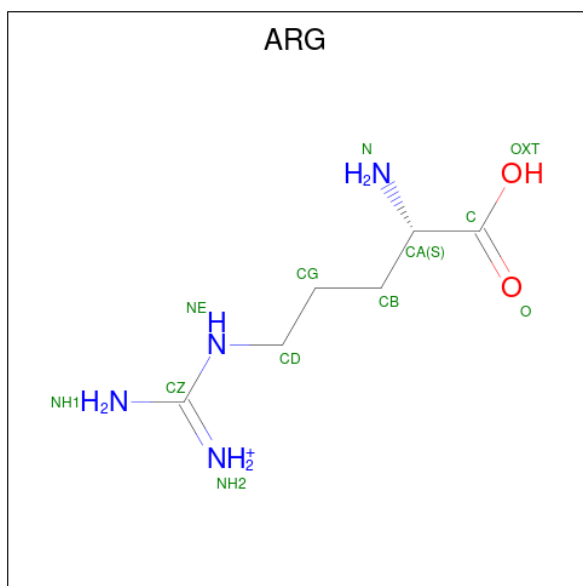
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

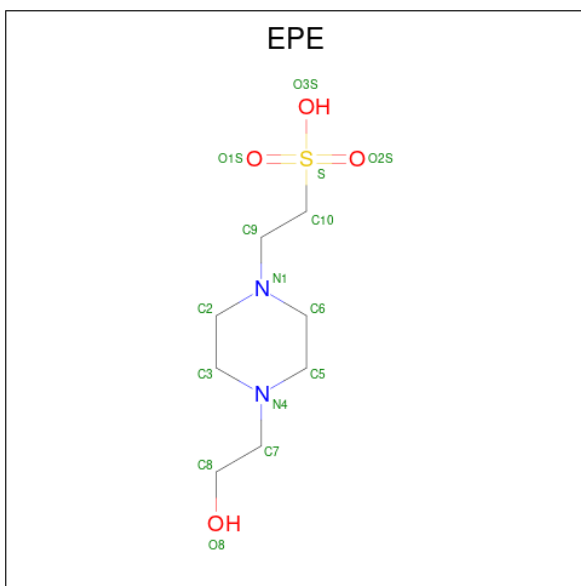
- Molecule 8 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			12	6	4	2		
8	B	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 9 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD

ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	165	Total	O	0	0
			165	165		
10	B	173	Total	O	0	0
			173	173		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.86Å 80.17Å 84.64Å 90.00° 115.50° 90.00°	Depositor
Resolution (Å)	76.39 – 2.01 76.39 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (76.39-2.01) 99.9 (76.39-2.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.02Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.195 , 0.246 0.201 , 0.255	Depositor DCC
R_{free} test set	2434 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4899	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, SO3, ACT, ZN, EDO, EPE, GOL

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	0.68	1/2236 (0.0%)	0.98	5/3009 (0.2%)
1	B	0.57	0/2244	0.94	1/3020 (0.0%)
All	All	0.63	1/4480 (0.0%)	0.96	6/6029 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	GLU	CD-OE1	17.96	1.59	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	GLU	CG-CD-OE1	7.49	135.63	118.40
1	A	274	GLU	CB-CG-CD	7.25	124.93	112.60
1	A	274	GLU	CG-CD-OE2	-7.20	101.84	118.40
1	A	274	GLU	CB-CA-C	6.52	121.61	110.79
1	B	257	ILE	N-CA-CB	-5.06	105.28	112.12
1	A	238	ARG	CG-CD-NE	5.04	123.09	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238	ARG	Sidechain
1	B	39	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2195	0	2305	54	3
1	B	2200	0	2309	43	1
2	A	6	0	0	0	0
2	B	3	0	0	0	0
3	A	24	0	0	16	1
3	B	8	0	0	4	0
4	A	18	0	24	4	0
4	B	12	0	16	6	0
5	A	14	0	20	3	0
5	B	14	0	20	1	0
6	A	12	0	18	3	0
6	B	12	0	18	1	0
7	A	4	0	3	0	0
8	A	12	0	12	6	1
8	B	12	0	12	8	1
9	B	15	0	17	1	0
10	A	165	0	0	13	0
10	B	173	0	0	10	0
All	All	4899	0	4774	100	4

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 11.

All (100) 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:188:GLU:OE1	8:A:322:ARG:NE	1.67	1.27
3:A:310:SO3:S	1:B:45:HIS:NE2	2.08	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ASP:OD2	3:B:304:SO3:S	1.97	1.22
1:A:278:ASP:OD2	3:A:307:SO3:S	1.98	1.20
1:A:80:ASP:OD1	3:A:311:SO3:S	2.04	1.16
1:B:188:GLU:OE1	8:B:313:ARG:NE	1.81	1.13
1:A:45:HIS:NE2	3:A:308:SO3:S	2.27	1.05
1:A:188:GLU:OE1	8:A:322:ARG:CZ	2.07	1.01
1:A:253:GLU:CD	3:A:310:SO3:O3	2.03	1.01
1:B:147:LYS:NZ	3:B:305:SO3:O1	1.94	1.00
3:A:308:SO3:O1	10:A:401:HOH:O	1.82	0.96
1:A:105:GLU:OE1	10:A:402:HOH:O	1.88	0.92
1:B:212:GLU:OE2	8:B:313:ARG:CA	2.19	0.90
1:A:222:GLU:OE1	3:A:309:SO3:S	2.32	0.88
1:A:205:ASP:OD2	3:A:312:SO3:S	2.33	0.87
1:B:222:GLU:OE2	3:B:305:SO3:S	2.33	0.86
1:A:238:ARG:NH2	10:A:404:HOH:O	2.11	0.83
1:B:122:GLU:OE2	10:B:402:HOH:O	1.96	0.82
1:A:280:GLU:OE1	1:A:284:LYS:NZ	2.13	0.80
1:A:188:GLU:OE1	8:A:322:ARG:NH2	2.14	0.79
1:B:205:ASP:OD1	4:B:306:GOL:H32	1.84	0.77
1:B:212:GLU:OE2	8:B:313:ARG:HA	1.85	0.76
1:B:188:GLU:OE1	8:B:313:ARG:CZ	2.34	0.75
1:A:188:GLU:CD	8:A:322:ARG:HE	1.95	0.74
1:B:212:GLU:OE2	8:B:313:ARG:N	2.20	0.74
1:B:117:ASP:OD1	10:B:403:HOH:O	2.05	0.73
1:A:151:GLU:OE1	10:A:403:HOH:O	2.07	0.72
1:A:27:LEU:HD12	1:A:75:LEU:HD22	1.72	0.72
1:B:188:GLU:CD	8:B:313:ARG:HE	1.98	0.71
1:A:251:LYS:NZ	4:A:313:GOL:O1	2.25	0.70
1:A:212:GLU:OE2	8:A:322:ARG:C	2.36	0.68
1:A:278:ASP:CG	3:A:307:SO3:S	2.77	0.68
1:A:95:ASP:OD2	5:A:316:PEG:O2	2.10	0.67
1:A:252:ASP:OD1	1:A:255:ARG:NH2	2.22	0.67
1:B:58:GLU:OE2	10:B:405:HOH:O	2.12	0.67
1:B:38:PRO:O	1:B:46:PHE:HE2	1.79	0.66
1:B:278:ASP:CG	3:B:304:SO3:S	2.78	0.66
1:A:253:GLU:OE2	3:A:310:SO3:O3	2.12	0.66
1:B:176:ARG:H	4:B:307:GOL:H32	1.60	0.65
1:A:246:MET:HG3	10:B:412:HOH:O	1.97	0.64
1:A:80:ASP:CG	3:A:311:SO3:S	2.81	0.63
1:A:245:HIS:CG	1:A:251:LYS:HD3	2.36	0.61
3:A:312:SO3:O3	10:A:405:HOH:O	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:308:PEG:H22	10:B:448:HOH:O	2.00	0.60
1:B:105:GLU:OE1	10:B:406:HOH:O	2.16	0.60
4:A:313:GOL:O3	10:A:406:HOH:O	2.16	0.60
1:B:212:GLU:CD	8:B:313:ARG:HA	2.27	0.60
1:A:42:ILE:HD13	1:B:253:GLU:HG3	1.84	0.60
1:A:175:SER:HB2	4:A:315:GOL:H12	1.84	0.59
1:A:238:ARG:NH2	1:A:242:ASP:OD2	2.35	0.59
1:B:238:ARG:NH2	1:B:242:ASP:OD2	2.36	0.58
1:B:23:MET:HE3	1:B:48:ILE:HA	1.85	0.58
1:A:164:ARG:NH2	10:A:413:HOH:O	2.37	0.58
1:A:23:MET:HE3	1:A:48:ILE:HA	1.85	0.57
1:B:243:SER:HB3	10:B:497:HOH:O	2.04	0.57
8:A:322:ARG:OXT	10:A:407:HOH:O	2.17	0.56
1:A:245:HIS:CE1	6:A:318:EDO:H22	2.41	0.56
1:A:137:ILE:HG22	6:A:320:EDO:H21	1.86	0.56
1:A:205:ASP:CG	3:A:312:SO3:S	2.89	0.55
1:A:280:GLU:HG2	1:A:284:LYS:HE2	1.87	0.55
1:B:136:LYS:NZ	10:B:417:HOH:O	2.37	0.55
1:A:253:GLU:CG	3:A:310:SO3:O3	2.55	0.55
1:B:176:ARG:HE	4:B:307:GOL:H11	1.70	0.54
1:B:217:LYS:NZ	10:B:407:HOH:O	2.19	0.54
1:B:39:ARG:HD2	9:B:314:EPE:H101	1.91	0.53
1:B:95:ASP:HB2	6:B:311:EDO:H11	1.91	0.53
3:A:310:SO3:S	1:B:45:HIS:CD2	2.99	0.53
1:A:245:HIS:CG	1:A:251:LYS:CD	2.93	0.51
1:A:112:LYS:NZ	10:A:415:HOH:O	2.38	0.49
1:B:188:GLU:CD	8:B:313:ARG:NE	2.63	0.49
1:B:245:HIS:ND1	10:B:404:HOH:O	2.09	0.49
1:B:37:ARG:HD3	1:B:39:ARG:O	2.12	0.48
1:A:27:LEU:CD1	1:A:75:LEU:HD22	2.41	0.48
1:A:144:LYS:O	1:A:148:THR:HG23	2.13	0.48
1:A:241:LYS:HE3	4:A:313:GOL:H2	1.95	0.48
1:B:38:PRO:O	1:B:46:PHE:CE2	2.62	0.48
1:A:45:HIS:CD2	3:A:308:SO3:S	3.05	0.48
1:B:144:LYS:O	1:B:148:THR:HG23	2.14	0.47
1:A:245:HIS:CD2	1:A:251:LYS:HD3	2.50	0.46
1:A:95:ASP:OD2	5:A:316:PEG:H42	2.15	0.46
1:A:280:GLU:O	1:A:284:LYS:HG3	2.16	0.46
1:A:95:ASP:OD1	5:A:316:PEG:H12	2.16	0.46
1:A:46:PHE:O	1:A:198:PHE:HA	2.16	0.45
1:A:147:LYS:NZ	10:A:420:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:SER:HB2	4:B:307:GOL:H31	1.97	0.45
1:B:205:ASP:OD2	4:B:306:GOL:C1	2.66	0.44
1:A:39:ARG:O	1:A:39:ARG:HD2	2.17	0.44
1:A:238:ARG:HD2	10:A:527:HOH:O	2.19	0.43
1:A:238:ARG:CG	1:A:238:ARG:HH21	2.32	0.43
1:A:36:ILE:HD13	1:A:101:ILE:CD1	2.48	0.42
1:B:46:PHE:O	1:B:198:PHE:HA	2.18	0.42
10:A:422:HOH:O	1:B:164:ARG:NH1	2.54	0.41
1:B:165:MET:HE1	1:B:211:ILE:HD11	2.02	0.41
1:B:155:VAL:HG23	1:B:157:TYR:CE2	2.56	0.41
1:A:39:ARG:HB3	1:A:44:GLN:HB2	2.03	0.41
1:A:117:ASP:OD1	6:A:320:EDO:O1	2.35	0.41
1:A:217:LYS:NZ	10:A:429:HOH:O	2.53	0.41
1:B:241:LYS:O	1:B:244:ILE:HG23	2.20	0.41
1:A:230:GLN:NE2	1:B:230:GLN:OE1	2.54	0.40
1:B:175:SER:HB2	4:B:307:GOL:C3	2.51	0.40

All (4) 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:B:286:HIS:NE2	8:A:322:ARG:NE[4_556]	2.08	0.12
1:A:199:TYR:OH	1:A:274:GLU:OE1[4_556]	2.09	0.11
1:A:286:HIS:NE2	8:B:313:ARG:NE[4_545]	2.14	0.06
1:A:24:ARG:NH1	3:A:307:SO3:O1[4_556]	2.19	0.01

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	268/290 (92%)	265 (99%)	3 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	269/290 (93%)	267 (99%)	2 (1%)	0	100	100
All	All	537/580 (93%)	532 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	243/261 (93%)	234 (96%)	9 (4%)	30	30
1	B	244/261 (94%)	234 (96%)	10 (4%)	27	26
All	All	487/522 (93%)	468 (96%)	19 (4%)	28	28

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	MET
1	A	37	ARG
1	A	39	ARG
1	A	136	LYS
1	A	178	SER
1	A	188	GLU
1	A	203	LYS
1	A	230	GLN
1	A	246	MET
1	B	23	MET
1	B	37	ARG
1	B	42	ILE
1	B	75	LEU
1	B	97	LYS
1	B	125	LYS
1	B	168	LYS
1	B	178	SER
1	B	215	LYS

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Mol	Chain	Res	Type
1	B	257	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	B	186	ASN
1	B	230	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 36 ligands modelled in this entry, 9 are monoatomic - leaving 27 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	$\# Z > 2$
3	SO3	B	304	-	1,3,3	1.08	0	0,3,3	-	-
5	PEG	A	317	-	6,6,6	0.16	0	5,5,5	0.07	0
6	EDO	A	319	-	3,3,3	0.18	0	2,2,2	0.26	0
3	SO3	A	312	-	1,3,3	1.44	0	0,3,3	-	-
6	EDO	B	310	-	3,3,3	0.19	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	A	316	-	6,6,6	0.26	0	5,5,5	0.11	0
3	SO3	A	311	-	1,3,3	6.66	1 (100%)	0,3,3	-	-
5	PEG	B	308	-	6,6,6	0.16	0	5,5,5	0.08	0
5	PEG	B	309	-	6,6,6	0.19	0	5,5,5	0.15	0
8	ARG	B	313	-	10,11,11	1.18	1 (10%)	9,13,13	3.54	4 (44%)
4	GOL	A	314	-	5,5,5	0.12	0	5,5,5	0.32	0
3	SO3	A	309	-	1,3,3	2.30	1 (100%)	0,3,3	-	-
3	SO3	A	307	-	1,3,3	2.58	1 (100%)	0,3,3	-	-
4	GOL	B	306	-	5,5,5	0.09	0	5,5,5	0.34	0
6	EDO	B	312	-	3,3,3	0.20	0	2,2,2	0.21	0
9	EPE	B	314	-	15,15,15	1.03	1 (6%)	19,20,20	1.36	3 (15%)
6	EDO	A	320	-	3,3,3	0.14	0	2,2,2	0.08	0
3	SO3	A	310	-	1,3,3	5.04	1 (100%)	0,3,3	-	-
4	GOL	A	313	-	5,5,5	0.14	0	5,5,5	0.33	0
8	ARG	A	322	-	10,11,11	0.81	1 (10%)	9,13,13	1.02	1 (11%)
7	ACT	A	321	-	3,3,3	1.28	0	3,3,3	0.74	0
4	GOL	A	315	-	5,5,5	0.48	0	5,5,5	0.89	0
4	GOL	B	307	-	5,5,5	0.32	0	5,5,5	0.58	0
3	SO3	A	308	-	1,3,3	1.36	0	0,3,3	-	-
6	EDO	B	311	-	3,3,3	0.13	0	2,2,2	0.33	0
6	EDO	A	318	-	3,3,3	0.21	0	2,2,2	0.56	0
3	SO3	B	305	-	1,3,3	1.36	0	0,3,3	-	-

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
5	PEG	B	308	-	-	2/4/4/4	-
5	PEG	B	309	-	-	3/4/4/4	-
4	GOL	B	307	-	-	4/4/4/4	-
8	ARG	B	313	-	-	0/11/11/11	-
5	PEG	A	317	-	-	2/4/4/4	-
9	EPE	B	314	-	-	5/9/19/19	0/1/1/1
6	EDO	A	320	-	-	0/1/1/1	-
6	EDO	A	319	-	-	1/1/1/1	-
6	EDO	B	312	-	-	0/1/1/1	-
4	GOL	A	314	-	-	4/4/4/4	-
6	EDO	B	311	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	313	-	-	1/4/4/4	-
8	ARG	A	322	-	-	0/11/11/11	-
6	EDO	B	310	-	-	0/1/1/1	-
6	EDO	A	318	-	-	1/1/1/1	-
4	GOL	A	315	-	-	0/4/4/4	-
5	PEG	A	316	-	-	2/4/4/4	-
4	GOL	B	306	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	311	SO3	O1-S	6.66	1.72	1.44
3	A	310	SO3	O1-S	5.04	1.65	1.44
9	B	314	EPE	O1S-S	3.68	1.55	1.45
3	A	307	SO3	O1-S	2.58	1.55	1.44
3	A	309	SO3	O1-S	2.30	1.54	1.44
8	B	313	ARG	O-C	2.25	1.28	1.22
8	A	322	ARG	OXT-C	-2.06	1.24	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	313	ARG	CG-CD-NE	7.66	133.67	112.20
8	B	313	ARG	CB-CA-C	5.17	124.15	110.45
8	B	313	ARG	CB-CG-CD	3.96	123.51	112.07
9	B	314	EPE	O3S-S-O2S	3.61	120.43	111.40
9	B	314	EPE	O2S-S-O1S	-2.80	104.73	113.82
8	A	322	ARG	CG-CD-NE	2.51	119.24	112.20
8	B	313	ARG	NE-CZ-NH2	2.39	124.77	120.67
9	B	314	EPE	O1S-S-C10	-2.36	103.17	106.73

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	307	GOL	O1-C1-C2-O2
4	B	307	GOL	O1-C1-C2-C3
9	B	314	EPE	S-C10-C9-N1
5	A	316	PEG	O2-C3-C4-O4
5	A	317	PEG	O1-C1-C2-O2
9	B	314	EPE	C9-C10-S-O3S

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Mol	Chain	Res	Type	Atoms
5	A	316	PEG	O1-C1-C2-O2
5	A	317	PEG	O2-C3-C4-O4
5	B	309	PEG	O1-C1-C2-O2
5	B	309	PEG	O2-C3-C4-O4
4	A	314	GOL	O1-C1-C2-C3
4	A	314	GOL	C1-C2-C3-O3
4	B	307	GOL	C1-C2-C3-O3
5	B	308	PEG	O2-C3-C4-O4
6	A	319	EDO	O1-C1-C2-O2
5	B	308	PEG	O1-C1-C2-O2
4	A	314	GOL	O2-C2-C3-O3
4	B	306	GOL	O1-C1-C2-O2
9	B	314	EPE	C10-C9-N1-C2
9	B	314	EPE	C10-C9-N1-C6
4	B	307	GOL	O2-C2-C3-O3
9	B	314	EPE	C9-C10-S-O1S
4	B	306	GOL	O1-C1-C2-C3
5	B	309	PEG	C4-C3-O2-C2
6	A	318	EDO	O1-C1-C2-O2
4	A	313	GOL	O1-C1-C2-C3
4	A	314	GOL	O1-C1-C2-O2

There are no ring outliers.

20 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	304	SO3	2	0
3	A	312	SO3	3	0
5	A	316	PEG	3	0
3	A	311	SO3	2	0
5	B	308	PEG	1	0
8	B	313	ARG	8	1
3	A	309	SO3	1	0
3	A	307	SO3	2	1
4	B	306	GOL	2	0
9	B	314	EPE	1	0
6	A	320	EDO	2	0
3	A	310	SO3	5	0
4	A	313	GOL	3	0
8	A	322	ARG	6	1
4	A	315	GOL	1	0
4	B	307	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	308	SO3	3	0
6	B	311	EDO	1	0
6	A	318	EDO	1	0
3	B	305	SO3	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 ⓘ

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	270/290 (93%)	0.43	20 (7%)	20 19	19, 29, 57, 124	0
1	B	270/290 (93%)	0.37	17 (6%)	26 24	17, 30, 51, 72	1 (0%)
All	All	540/580 (93%)	0.40	37 (6%)	23 21	17, 30, 54, 124	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	SER	7.0
1	A	42	ILE	6.8
1	A	38	PRO	6.1
1	A	199	TYR	5.0
1	A	43	GLY	4.3
1	B	254	ILE	3.4
1	A	21	SER	3.1
1	A	22	LYS	3.0
1	A	39	ARG	2.9
1	B	289	ILE	2.9
1	A	40	ASP	2.8
1	A	37	ARG	2.8
1	B	290	SER	2.8
1	B	40	ASP	2.7
1	A	35	GLY	2.7
1	B	42	ILE	2.7
1	B	21	SER	2.6
1	A	48	ILE	2.5
1	A	216	ASP	2.5
1	B	253	GLU	2.5
1	A	265	ASN	2.5
1	B	257	ILE	2.4
1	A	290	SER	2.4
1	B	246	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	250	SER	2.4
1	B	244	ILE	2.4
1	A	119	VAL	2.3
1	B	247	LEU	2.3
1	B	248	GLY	2.3
1	A	44	GLN	2.2
1	B	133	ILE	2.2
1	A	58	GLU	2.1
1	A	45	HIS	2.1
1	B	43	GLY	2.1
1	A	94	ILE	2.1
1	B	51	ASP	2.0
1	B	216	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	ACT	A	321	4/4	0.69	0.24	41,46,48,51	0
9	EPE	B	314	15/15	0.70	0.24	50,65,83,88	0
5	PEG	B	308	7/7	0.76	0.16	57,63,76,82	0
6	EDO	A	320	4/4	0.77	0.22	53,58,65,67	0
4	GOL	A	313	6/6	0.80	0.16	46,49,52,53	0
6	EDO	B	310	4/4	0.80	0.18	60,64,65,65	0
4	GOL	B	306	6/6	0.81	0.16	44,50,51,53	0
6	EDO	B	312	4/4	0.81	0.13	58,59,60,62	0
3	SO3	B	305	4/4	0.82	0.16	41,44,46,47	0
6	EDO	B	311	4/4	0.83	0.18	47,48,51,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	A	317	7/7	0.83	0.20	65,72,80,83	0
3	SO3	A	312	4/4	0.85	0.10	55,64,65,69	0
4	GOL	A	314	6/6	0.86	0.12	58,58,61,61	0
6	EDO	A	319	4/4	0.86	0.14	42,44,47,50	0
4	GOL	A	315	6/6	0.87	0.15	27,34,40,45	0
5	PEG	B	309	7/7	0.88	0.15	44,52,58,58	0
5	PEG	A	316	7/7	0.88	0.17	29,37,45,57	0
3	SO3	A	309	4/4	0.88	0.13	23,31,32,35	0
8	ARG	A	322	12/12	0.88	0.16	15,38,48,59	0
3	SO3	A	311	4/4	0.88	0.13	20,20,27,30	0
8	ARG	B	313	12/12	0.89	0.17	8,23,38,39	0
4	GOL	B	307	6/6	0.90	0.11	22,28,37,38	0
3	SO3	A	308	4/4	0.92	0.09	50,50,53,57	0
3	SO3	B	304	4/4	0.92	0.11	29,36,40,44	0
6	EDO	A	318	4/4	0.92	0.12	32,32,36,36	0
3	SO3	A	310	4/4	0.95	0.09	16,17,21,23	0
3	SO3	A	307	4/4	0.95	0.08	24,26,32,34	0
2	ZN	A	304	1/1	0.96	0.06	78,78,78,78	0
2	ZN	B	303	1/1	0.98	0.03	36,36,36,36	0
2	ZN	A	302	1/1	0.98	0.05	42,42,42,42	0
2	ZN	A	306	1/1	0.98	0.04	55,55,55,55	0
2	ZN	B	301	1/1	0.98	0.09	57,57,57,57	0
2	ZN	A	305	1/1	0.99	0.02	28,28,28,28	0
2	ZN	A	303	1/1	0.99	0.03	31,31,31,31	0
2	ZN	A	301	1/1	0.99	0.03	34,34,34,34	0
2	ZN	B	302	1/1	0.99	0.03	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.