



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2025 – 01:29 pm BST

PDB ID : 9FMQ / pdb_00009fmq
Title : Crystal structure of C. merolae LAMMER-like dual specificity kinase (CmLIK) hairpin mutant kinase domain
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Deposited on : 2024-06-06
Resolution : 1.77 Å(reported)

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

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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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

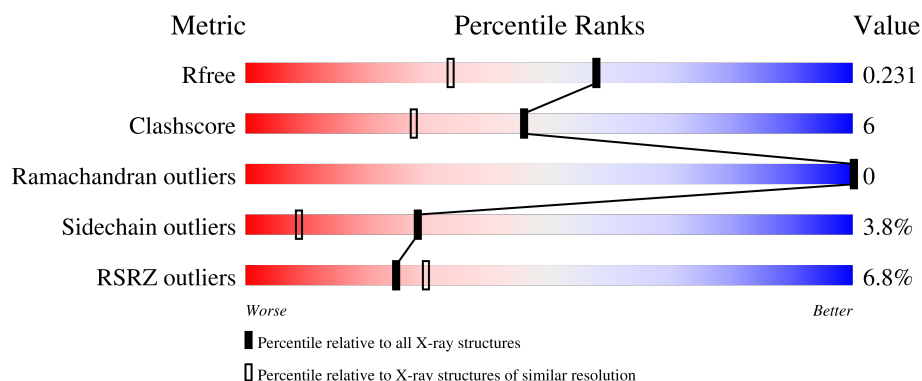
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

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	384	<div> <div>6%</div> <div>79%</div> <div>13%</div> <div>8%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3022 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 LAMMER-like dual specificity kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	5	0
			2898	1837	540	506	15			

There are 25 discrepancies between the modelled and reference sequences:

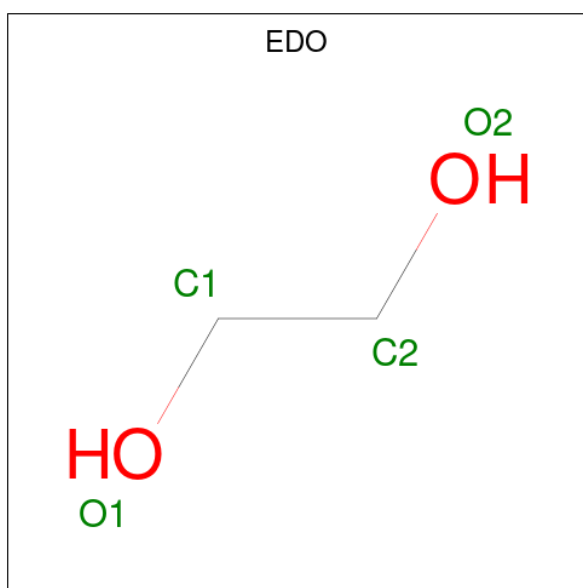
Chain	Residue	Modelled	Actual	Comment	Reference
A	440	GLY	-	expression tag	UNP M1UWB5
A	441	PRO	-	expression tag	UNP M1UWB5
A	442	LEU	-	expression tag	UNP M1UWB5
A	443	GLY	-	expression tag	UNP M1UWB5
A	444	SER	-	expression tag	UNP M1UWB5
A	445	PRO	-	expression tag	UNP M1UWB5
A	446	GLU	-	expression tag	UNP M1UWB5
A	447	PHE	-	expression tag	UNP M1UWB5
A	610	LYS	PRO	engineered mutation	UNP M1UWB5
A	612	ASP	SER	engineered mutation	UNP M1UWB5
A	614	THR	-	insertion	UNP M1UWB5
A	615	GLU	-	insertion	UNP M1UWB5
A	616	ALA	-	insertion	UNP M1UWB5
A	618	ASN	-	insertion	UNP M1UWB5
A	620	LYS	-	insertion	UNP M1UWB5
A	621	MET	-	insertion	UNP M1UWB5
A	622	LYS	ASN	engineered mutation	UNP M1UWB5
A	624	ASP	GLN	engineered mutation	UNP M1UWB5
A	625	GLU	ILE	engineered mutation	UNP M1UWB5
A	626	ARG	THR	engineered mutation	UNP M1UWB5
A	627	THR	GLU	engineered mutation	UNP M1UWB5
A	628	ILE	HIS	engineered mutation	UNP M1UWB5
A	630	ASN	-	insertion	UNP M1UWB5
A	631	PRO	-	insertion	UNP M1UWB5
A	632	ASP	GLN	engineered mutation	UNP M1UWB5

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

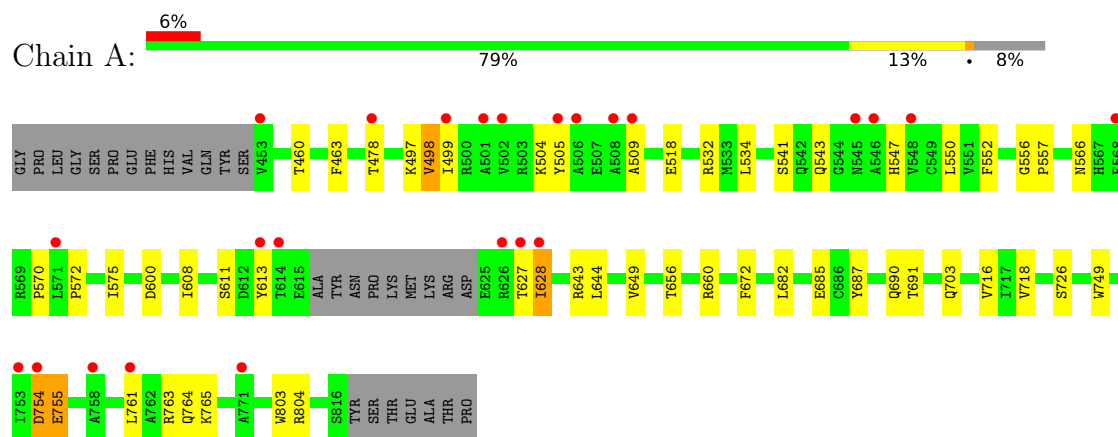
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	83	Total O 83 83	0	0

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: LAMMER-like dual specificity kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.72Å 68.67Å 84.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.36 – 1.77 42.36 – 1.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.36-1.77) 99.9 (42.36-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.77Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.192 , 0.230 0.192 , 0.231	Depositor DCC
R_{free} test set	1889 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3022	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.93% 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: ACT, EDO, CA

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	0.46	0/2973	0.63	0/4026

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	2898	0	2923	34	0
2	A	8	0	6	1	0
3	A	32	0	48	6	0
4	A	1	0	0	0	0
5	A	83	0	0	0	0
All	All	3022	0	2977	34	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 (34) 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:755:GLU:H	1:A:763:ARG:NH2	1.90	0.69
1:A:660:ARG:HH12	3:A:905:EDO:H12	1.58	0.67
1:A:541:SER:OG	1:A:543:GLN:OE1	2.12	0.65
1:A:755:GLU:H	1:A:763:ARG:HH21	1.46	0.64
1:A:804:ARG:HA	3:A:909:EDO:H12	1.86	0.57
1:A:499:ILE:HG13	1:A:509:ALA:HB2	1.86	0.57
1:A:685[B]:GLU:HG2	1:A:690:GLN:O	2.05	0.56
1:A:803:TRP:HA	3:A:908:EDO:H11	1.90	0.54
1:A:460:THR:CG2	1:A:463:PHE:H	2.21	0.53
1:A:534:LEU:O	2:A:902:ACT:C	2.56	0.53
1:A:685[B]:GLU:HG2	1:A:691:THR:HA	1.90	0.53
1:A:572:PRO:HD2	1:A:575:ILE:HD12	1.90	0.53
1:A:600:ASP:OD1	1:A:656:THR:HG23	2.10	0.52
1:A:754:ASP:HB3	1:A:763:ARG:HH21	1.76	0.50
1:A:556:GLY:O	3:A:903:EDO:H21	2.12	0.50
1:A:518:GLU:OE1	1:A:643:ARG:NH2	2.41	0.50
1:A:499:ILE:HG13	1:A:509:ALA:CB	2.42	0.49
1:A:608:ILE:N	1:A:608:ILE:HD12	2.28	0.48
1:A:518:GLU:OE1	1:A:643:ARG:NH1	2.47	0.47
1:A:532:ARG:HA	1:A:532:ARG:HD2	1.79	0.47
1:A:478:THR:HB	1:A:505:TYR:CZ	2.50	0.47
1:A:611:SER:HB3	1:A:613:TYR:CZ	2.51	0.46
1:A:498:VAL:HG23	1:A:547:HIS:HB3	1.99	0.45
1:A:552:PHE:CZ	3:A:910:EDO:H21	2.51	0.45
1:A:557:PRO:HD2	1:A:608:ILE:O	2.16	0.45
1:A:460:THR:HG23	1:A:463:PHE:H	1.81	0.45
1:A:570:PRO:HB3	1:A:687:TYR:O	2.18	0.43
1:A:703:GLN:HG2	1:A:749:TRP:CD2	2.53	0.43
1:A:761:LEU:O	1:A:765:LYS:HG3	2.19	0.42
1:A:682:LEU:C	1:A:682:LEU:HD23	2.45	0.42
1:A:613:TYR:HE1	1:A:628:ILE:HD13	1.84	0.41
1:A:644:LEU:HB2	1:A:672:PHE:CZ	2.55	0.41
1:A:550:LEU:HD12	1:A:550:LEU:N	2.36	0.41
1:A:497:LYS:NZ	3:A:910:EDO:H12	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	356/384 (93%)	345 (97%)	11 (3%)	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	320/340 (94%)	308 (96%)	12 (4%)	28	9

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	VAL
1	A	504	LYS
1	A	566	ASN
1	A	627	THR
1	A	628	ILE
1	A	649	VAL
1	A	716	VAL
1	A	718	VAL
1	A	726	SER
1	A	754	ASP
1	A	755	GLU
1	A	764	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	696	HIS

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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	EDO	A	903	-	3,3,3	0.53	0	2,2,2	0.40	0
3	EDO	A	907	-	3,3,3	0.52	0	2,2,2	0.40	0
3	EDO	A	910	-	3,3,3	0.65	0	2,2,2	0.84	0
3	EDO	A	906	-	3,3,3	0.70	0	2,2,2	0.07	0
3	EDO	A	909	-	3,3,3	0.77	0	2,2,2	0.35	0
3	EDO	A	908	-	3,3,3	0.51	0	2,2,2	0.12	0
2	ACT	A	902	-	3,3,3	1.45	1 (33%)	3,3,3	1.37	0
2	ACT	A	901	-	3,3,3	2.05	1 (33%)	3,3,3	1.26	0
3	EDO	A	904	-	3,3,3	0.54	0	2,2,2	0.35	0
3	EDO	A	905	-	3,3,3	0.59	0	2,2,2	0.04	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
3	EDO	A	903	-	-	1/1/1/1	-
3	EDO	A	907	-	-	0/1/1/1	-
3	EDO	A	910	-	-	0/1/1/1	-
3	EDO	A	906	-	-	0/1/1/1	-
3	EDO	A	909	-	-	1/1/1/1	-
3	EDO	A	908	-	-	0/1/1/1	-
3	EDO	A	904	-	-	0/1/1/1	-
3	EDO	A	905	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ACT	CH3-C	3.04	1.61	1.49
2	A	902	ACT	CH3-C	2.23	1.58	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	903	EDO	O1-C1-C2-O2
3	A	909	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	903	EDO	1	0
3	A	910	EDO	2	0
3	A	909	EDO	1	0
3	A	908	EDO	1	0
2	A	902	ACT	1	0
3	A	905	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	355/384 (92%)	0.46	24 (6%)	25 30	21, 49, 98, 137	5 (1%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	502	VAL	4.6
1	A	453	VAL	3.7
1	A	627	THR	3.5
1	A	613	TYR	3.5
1	A	758	ALA	3.0
1	A	501	ALA	2.9
1	A	546	ALA	2.9
1	A	568	PHE	2.7
1	A	761	LEU	2.7
1	A	508	ALA	2.7
1	A	628	ILE	2.6
1	A	614	THR	2.4
1	A	509	ALA	2.4
1	A	478	THR	2.3
1	A	571	LEU	2.3
1	A	505	TYR	2.3
1	A	771	ALA	2.2
1	A	506	ALA	2.2
1	A	626	ARG	2.1
1	A	548	VAL	2.1
1	A	545	ASN	2.1
1	A	753	ILE	2.1
1	A	499	ILE	2.1
1	A	754	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 monosaccharides 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	ACT	A	901	4/4	0.56	0.22	54,61,64,68	0
3	EDO	A	904	4/4	0.67	0.16	66,67,69,75	0
2	ACT	A	902	4/4	0.69	0.16	61,61,70,71	0
3	EDO	A	905	4/4	0.74	0.14	52,55,61,62	0
3	EDO	A	906	4/4	0.75	0.19	56,58,58,60	0
3	EDO	A	903	4/4	0.79	0.14	60,62,64,68	0
3	EDO	A	910	4/4	0.81	0.16	49,52,52,58	0
3	EDO	A	908	4/4	0.86	0.11	54,56,58,60	0
3	EDO	A	909	4/4	0.90	0.12	46,48,48,54	0
3	EDO	A	907	4/4	0.90	0.10	42,49,51,57	0
4	CA	A	911	1/1	0.96	0.08	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.