



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 04:14 am GMT

PDB ID : 6H57
Title : Crystal structure of *S. cerevisiae* DEAH-box RNA helicase Dhr1, essential for small ribosomal subunit biogenesis
Authors : Roychowdhury, A.; Graille, M.
Deposited on : 2018-07-24
Resolution : 2.30 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

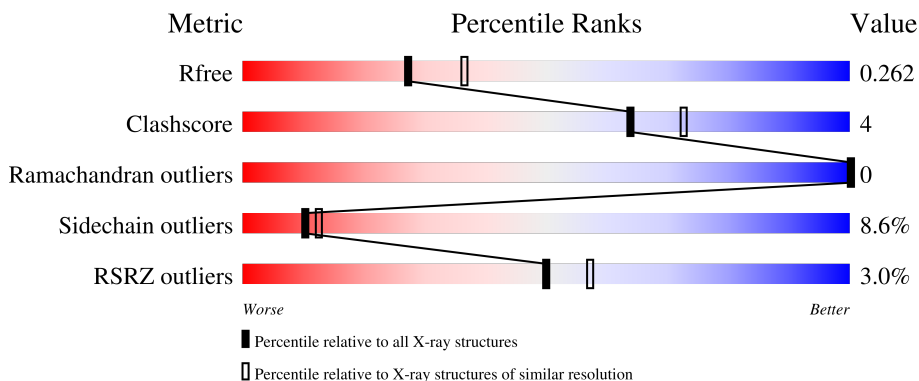
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	1267	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6697 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 ATP-dependent RNA helicase DHR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	795	6362	4069	1098	1160	35	0	3	0

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



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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

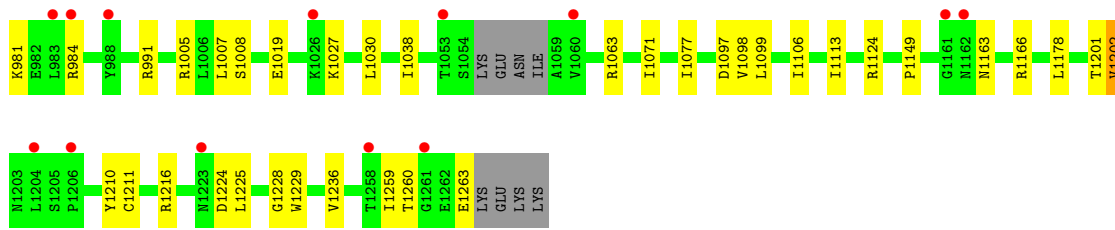
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Cl 4 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	274	Total O 274 274	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	57.31Å 115.80Å 157.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 2.30 48.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.83-2.30) 96.7 (48.83-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.29Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.205 , 0.245 0.216 , 0.262	Depositor DCC
R_{free} test set	2174 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtrriage
Anisotropy	0.367	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6697	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: MG, EDO, 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	0.49	0/6496	0.69	0/8767

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	6362	0	6501	54	0
2	A	56	0	84	9	0
3	A	1	0	0	0	0
4	A	4	0	0	0	0
5	A	274	0	0	0	0
All	All	6697	0	6585	54	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 4.

All (54) 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:595:ASN:HD21	1:A:609:LYS:HZ2	1.21	0.88
1:A:614:HIS:HD2	1:A:755:ARG:HD2	1.49	0.77
1:A:595:ASN:HD21	1:A:609:LYS:NZ	1.82	0.77
1:A:405:HIS:HB2	2:A:1305:EDO:H12	1.71	0.71
1:A:1149:PRO:HA	2:A:1301:EDO:H12	1.77	0.65
1:A:878:LYS:HG2	2:A:1309:EDO:H12	1.80	0.64
1:A:745:ARG:O	1:A:748:GLN:HG2	2.05	0.56
1:A:881:GLN:HG2	2:A:1308:EDO:H22	1.89	0.53
1:A:848:GLU:HG2	1:A:909:PRO:HD2	1.91	0.53
1:A:1149:PRO:CA	2:A:1301:EDO:H12	2.40	0.52
1:A:606:ALA:HB3	1:A:635:MET:HE1	1.92	0.52
1:A:795:SER:HB2	1:A:797:GLU:HG2	1.92	0.51
1:A:772:GLY:H	1:A:816:THR:HG21	1.75	0.51
1:A:614:HIS:CD2	1:A:755:ARG:HD2	2.40	0.50
1:A:442:PRO:HD2	1:A:551:LYS:HG2	1.93	0.49
1:A:1099:LEU:HD11	1:A:1229:TRP:HB3	1.94	0.49
1:A:563:ARG:CD	1:A:804:ALA:HB1	2.43	0.49
1:A:607:PHE:CZ	1:A:642:GLU:HG3	2.46	0.49
1:A:607:PHE:HZ	1:A:642:GLU:HG3	1.77	0.48
1:A:615:GLN:HG2	1:A:725:ALA:O	2.14	0.47
1:A:1228:GLY:H	2:A:1304:EDO:H22	1.79	0.47
1:A:475:TYR:HA	1:A:491:PHE:O	2.14	0.47
1:A:618:PRO:HA	1:A:723:GLN:HE22	1.81	0.46
1:A:847:VAL:HA	1:A:850:ILE:HD12	1.98	0.46
1:A:385:GLN:O	1:A:389:ILE:HG12	2.16	0.46
1:A:1202:VAL:HG13	1:A:1210:TYR:HB2	1.97	0.46
1:A:1216:ARG:HH22	2:A:1304:EDO:H11	1.81	0.46
1:A:788:ASN:HB3	1:A:791:ASN:HB2	1.97	0.46
1:A:609:LYS:HD3	1:A:822:TYR:HB3	1.98	0.45
1:A:1201:THR:HG23	1:A:1211:CYS:HB3	1.98	0.45
1:A:1124:ARG:HB2	1:A:1225:LEU:HA	1.99	0.45
1:A:933:ALA:HA	1:A:1038:ILE:HG12	1.99	0.45
1:A:1113:ILE:HB	1:A:1166:ARG:HH12	1.82	0.45
1:A:842:ILE:HG23	1:A:843:LEU:HD13	1.99	0.45
1:A:855:LYS:HE2	1:A:862:ILE:HD13	1.98	0.44
1:A:536:VAL:HG21	1:A:555:LEU:HB2	1.99	0.44
1:A:378:VAL:HG11	1:A:466:LEU:HD12	1.99	0.44
1:A:1124:ARG:HD3	1:A:1224:ASP:O	2.17	0.44
1:A:607:PHE:CE1	1:A:638:ARG:HG2	2.52	0.44
1:A:614:HIS:HE1	1:A:727:ASP:O	2.00	0.44
1:A:762:ASN:O	1:A:765:GLU:HB2	2.18	0.44
1:A:882:LEU:HB2	2:A:1309:EDO:H21	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:924:LEU:O	1:A:928:VAL:HG13	2.18	0.44
1:A:420:LYS:HE2	1:A:558:MET:HB3	2.00	0.43
1:A:728:PRO:HD2	1:A:753:GLY:O	2.18	0.43
1:A:1097:ASP:HB3	1:A:1106:ILE:HD12	2.01	0.43
1:A:454:ALA:O	1:A:458:MET:HB2	2.19	0.42
1:A:981:LYS:HA	1:A:984:ARG:HD3	2.00	0.42
1:A:809:ARG:O	1:A:812:ARG:HB2	2.20	0.42
1:A:503:HIS:HB2	2:A:1314:EDO:H22	2.02	0.42
1:A:614:HIS:CD2	1:A:755:ARG:HH21	2.37	0.41
1:A:943:GLU:C	1:A:945:GLU:H	2.22	0.41
1:A:563:ARG:HH22	1:A:808:GLN:HE21	1.69	0.41
1:A:901:LYS:O	1:A:904:LEU:HB2	2.21	0.41

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	790/1267 (62%)	772 (98%)	18 (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	712/1140 (62%)	651 (91%)	61 (9%)	10 12

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	375	TYR
1	A	382	ASP
1	A	386	LYS
1	A	389	ILE
1	A	391	LEU
1	A	437	ASP
1	A	466	LEU
1	A	472	LYS
1	A	480	ASP
1	A	482	THR
1	A	497	LEU
1	A	517	GLU
1	A	523	ILE
1	A	537	ARG
1	A	546	ASN
1	A	551	LYS
1	A	562	LEU
1	A	570	ASN
1	A	572	THR
1	A	587	GLN
1	A	601	ASN
1	A	604	ASP
1	A	609	LYS
1	A	710	GLU
1	A	736	SER
1	A	752	GLN
1	A	756	LEU
1	A	774	ARG
1	A	781	ARG
1	A	783	LYS
1	A	785	ARG
1	A	801	VAL
1	A	812	ARG
1	A	873	ARG
1	A	876	LEU
1	A	907	LEU
1	A	913	LYS
1	A	924	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	931	VAL
1	A	942	ASN
1	A	945	GLU
1	A	946	LEU
1	A	980	LYS
1	A	991	ARG
1	A	1005	ARG
1	A	1007	LEU
1	A	1008	SER
1	A	1019	GLU
1	A	1027	LYS
1	A	1030	LEU
1	A	1063	ARG
1	A	1071	ILE
1	A	1077	ILE
1	A	1098	VAL
1	A	1163	ASN
1	A	1178	LEU
1	A	1202	VAL
1	A	1236	VAL
1	A	1259	ILE
1	A	1260	THR
1	A	1263	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	476	GLN
1	A	546	ASN
1	A	570	ASN
1	A	595	ASN
1	A	601	ASN
1	A	614	HIS
1	A	723	GLN
1	A	808	GLN
1	A	942	ASN
1	A	1114	ASN
1	A	1163	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	EDO	A	1311	-	3,3,3	0.54	0	2,2,2	0.41	0
2	EDO	A	1303	-	3,3,3	0.51	0	2,2,2	0.36	0
2	EDO	A	1312	-	3,3,3	0.59	0	2,2,2	0.33	0
2	EDO	A	1309	-	3,3,3	0.44	0	2,2,2	0.60	0
2	EDO	A	1307	-	3,3,3	0.61	0	2,2,2	0.19	0
2	EDO	A	1313	-	3,3,3	0.62	0	2,2,2	0.13	0
2	EDO	A	1308	-	3,3,3	0.64	0	2,2,2	0.23	0
2	EDO	A	1301	-	3,3,3	0.45	0	2,2,2	0.38	0
2	EDO	A	1302	-	3,3,3	0.53	0	2,2,2	0.49	0
2	EDO	A	1304	-	3,3,3	0.62	0	2,2,2	0.37	0
2	EDO	A	1306	-	3,3,3	0.66	0	2,2,2	0.08	0
2	EDO	A	1310	-	3,3,3	0.69	0	2,2,2	0.40	0
2	EDO	A	1314	-	3,3,3	0.62	0	2,2,2	0.17	0
2	EDO	A	1305	-	3,3,3	0.59	0	2,2,2	0.17	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	EDO	A	1311	-	-	1/1/1/1	-
2	EDO	A	1303	-	-	0/1/1/1	-
2	EDO	A	1312	-	-	0/1/1/1	-
2	EDO	A	1309	-	-	1/1/1/1	-
2	EDO	A	1307	-	-	1/1/1/1	-
2	EDO	A	1313	-	-	0/1/1/1	-
2	EDO	A	1308	-	-	1/1/1/1	-
2	EDO	A	1301	-	-	0/1/1/1	-
2	EDO	A	1302	-	-	0/1/1/1	-
2	EDO	A	1304	-	-	0/1/1/1	-
2	EDO	A	1306	-	-	0/1/1/1	-
2	EDO	A	1310	-	-	0/1/1/1	-
2	EDO	A	1314	-	-	1/1/1/1	-
2	EDO	A	1305	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1314	EDO	O1-C1-C2-O2
2	A	1309	EDO	O1-C1-C2-O2
2	A	1311	EDO	O1-C1-C2-O2
2	A	1307	EDO	O1-C1-C2-O2
2	A	1308	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1309	EDO	2	0
2	A	1308	EDO	1	0
2	A	1301	EDO	2	0
2	A	1304	EDO	2	0
2	A	1314	EDO	1	0
2	A	1305	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	795/1267 (62%)	0.09	24 (3%) 50 57	24, 41, 72, 106	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1161	GLY	6.3
1	A	375	TYR	5.5
1	A	979	LEU	4.5
1	A	1026	LYS	4.0
1	A	983	LEU	3.8
1	A	984	ARG	3.6
1	A	373	ALA	3.6
1	A	1204	LEU	3.6
1	A	1206	PRO	3.5
1	A	1162	ASN	3.0
1	A	988	TYR	3.0
1	A	722	GLY	2.9
1	A	646	LYS	2.8
1	A	946	LEU	2.8
1	A	1053	THR	2.5
1	A	1261	GLY	2.5
1	A	947	GLY	2.5
1	A	1223[A]	ASN	2.5
1	A	374	PHE	2.4
1	A	978	GLU	2.3
1	A	1060	VAL	2.2
1	A	1258	THR	2.1
1	A	710	GLU	2.1
1	A	788	ASN	2.1

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 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	EDO	A	1306	4/4	0.61	0.23	56,58,61,63	0
2	EDO	A	1312	4/4	0.71	0.24	66,66,66,67	0
2	EDO	A	1308	4/4	0.75	0.34	59,60,60,60	0
2	EDO	A	1304	4/4	0.80	0.24	53,54,54,55	0
2	EDO	A	1310	4/4	0.83	0.20	45,47,48,49	0
4	CL	A	1318	1/1	0.83	0.14	80,80,80,80	0
2	EDO	A	1305	4/4	0.88	0.19	59,60,60,61	0
4	CL	A	1316	1/1	0.89	0.11	66,66,66,66	0
2	EDO	A	1311	4/4	0.91	0.19	45,47,50,51	0
2	EDO	A	1303	4/4	0.91	0.14	55,56,56,58	0
4	CL	A	1319	1/1	0.91	0.16	82,82,82,82	0
2	EDO	A	1314	4/4	0.92	0.18	57,57,57,58	0
2	EDO	A	1302	4/4	0.92	0.19	39,39,40,41	0
2	EDO	A	1307	4/4	0.93	0.19	45,46,48,48	0
2	EDO	A	1313	4/4	0.94	0.10	46,47,47,47	0
4	CL	A	1317	1/1	0.95	0.18	73,73,73,73	0
3	MG	A	1315	1/1	0.95	0.03	49,49,49,49	0
2	EDO	A	1309	4/4	0.95	0.25	36,36,38,39	0
2	EDO	A	1301	4/4	0.97	0.21	34,37,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.