



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:30 PM UTC

PDB ID : 4E7X / pdb_00004e7x
Title : Structural Basis for the Activity of a Cytoplasmic RNA Terminal U-transferase
Authors : Yates, L.A.; Fleurdepine, S.; Rissland, O.S.; DeColibus, L.; Harlos, K.; Norbury, C.J.; Gilbert, R.J.C.
Deposited on : 2012-03-19
Resolution : 3.20 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

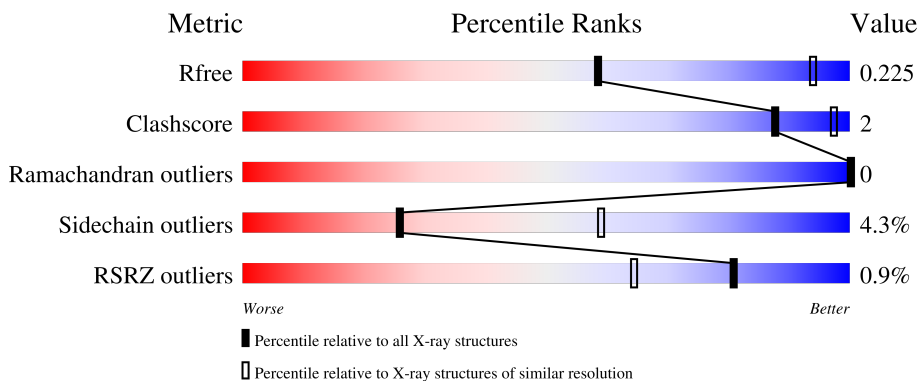
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	405	 71% 8% 21%
1	B	405	 69% 8% 23%
1	C	405	 69% 9% 22%
1	D	405	 71% 8% 21%

2 Entry composition [i](#)

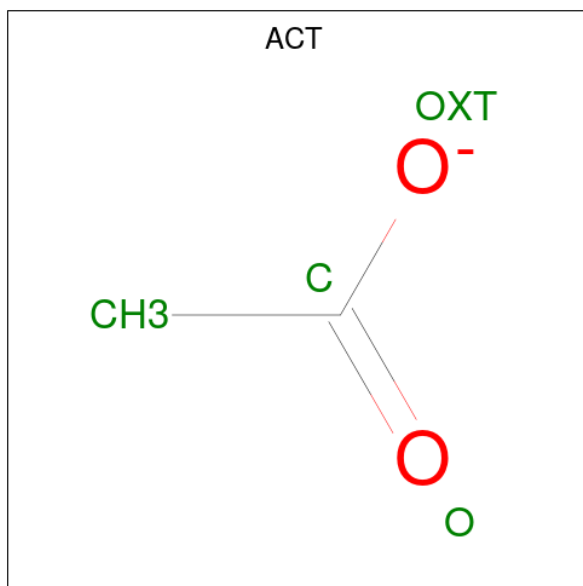
There are 3 unique types of molecules in this entry. The entry contains 10288 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Poly(A) RNA polymerase protein cid1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	Total 2589	C 1682	N 427	O 471	S 9	0	0	0
1	B	312	Total 2533	C 1649	N 417	O 458	S 9	0	0	0
1	C	316	Total 2553	C 1657	N 422	O 465	S 9	0	0	0
1	D	320	Total 2587	C 1678	N 430	O 470	S 9	0	0	0

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



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

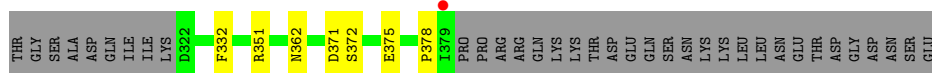
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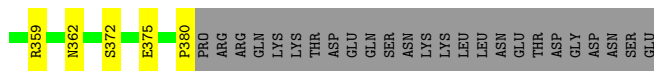
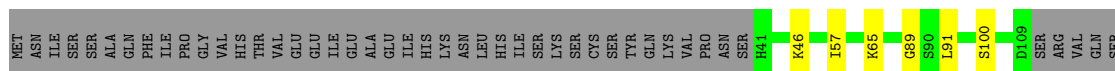
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

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



- Molecule 1: Poly(A) RNA polymerase protein cid1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.43Å 78.00Å 151.54Å 90.00° 109.45° 90.00°	Depositor
Resolution (Å)	64.27 – 3.20 64.27 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (64.27-3.20) 99.4 (64.27-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.19Å)	Xtrriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.179 , 0.213 0.186 , 0.225	Depositor DCC
R_{free} test set	1523 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtrriage
Anisotropy	0.100	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10288	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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

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	0.77	0/2650	1.26	5/3574 (0.1%)
1	B	0.80	1/2593 (0.0%)	1.25	3/3499 (0.1%)
1	C	0.78	1/2611 (0.0%)	1.25	6/3523 (0.2%)
1	D	0.79	0/2647	1.28	6/3573 (0.2%)
All	All	0.78	2/10501 (0.0%)	1.26	20/14169 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	302	GLN	CD-OE1	5.31	1.33	1.23
1	B	380	PRO	CA-C	5.29	1.55	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	116	THR	CA-C-N	6.61	129.51	120.46
1	C	116	THR	C-N-CA	6.61	129.51	120.46
1	D	380	PRO	N-CA-CB	6.27	109.90	103.00
1	A	116	THR	CA-C-N	5.91	128.86	120.53
1	A	116	THR	C-N-CA	5.91	128.86	120.53
1	B	89	GLY	CA-C-N	5.88	128.48	120.54
1	B	89	GLY	C-N-CA	5.88	128.48	120.54
1	C	89	GLY	CA-C-N	5.73	128.28	120.54
1	C	89	GLY	C-N-CA	5.73	128.28	120.54
1	B	84	GLU	CB-CG-CD	5.72	122.33	112.60
1	A	89	GLY	CA-C-N	5.70	128.24	120.54
1	A	89	GLY	C-N-CA	5.70	128.24	120.54
1	D	89	GLY	CA-C-N	5.61	128.11	120.54
1	D	89	GLY	C-N-CA	5.61	128.11	120.54
1	D	322	ASP	CA-CB-CG	5.37	117.97	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	ASN	CA-CB-CG	5.28	117.88	112.60
1	D	65	LYS	CA-C-N	5.17	127.16	120.44
1	D	65	LYS	C-N-CA	5.17	127.16	120.44
1	C	378	PRO	CA-C-N	5.12	130.91	121.70
1	C	378	PRO	C-N-CA	5.12	130.91	121.70

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	2589	0	2596	12	0
1	B	2533	0	2549	10	0
1	C	2553	0	2557	15	0
1	D	2587	0	2586	9	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	1	0
3	A	1	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
All	All	10288	0	10300	42	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 2.

All (42) 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:58:SER:HB3	1:C:261:PRO:HG3	1.64	0.78
1:A:58:SER:CB	1:C:261:PRO:HG3	2.15	0.76
1:A:325:ILE:HG22	1:A:347:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ARG:HH21	2:D:501:ACT:H1	1.63	0.63
1:B:363:SER:HB3	1:B:365:SER:HB3	1.84	0.60
1:D:256:LEU:HA	1:D:259:ILE:HD12	1.85	0.59
1:A:256:LEU:HA	1:A:259:ILE:HD12	1.84	0.58
1:A:58:SER:HB2	1:C:261:PRO:HG3	1.86	0.56
1:B:256:LEU:HA	1:B:259:ILE:HD12	1.86	0.56
1:C:256:LEU:HA	1:C:259:ILE:HD12	1.86	0.56
1:B:102:MET:HE2	1:B:104:LEU:HD21	1.90	0.53
1:B:101:ASP:OD1	1:B:158:GLN:HB3	2.09	0.52
1:A:75:CYS:HA	1:A:78:ARG:HD3	1.91	0.51
1:C:283:PHE:O	1:C:351:ARG:NH2	2.46	0.49
1:C:79:ILE:HD12	1:C:120:GLN:HB3	1.94	0.48
1:B:283:PHE:O	1:B:351:ARG:NH2	2.47	0.48
1:B:284:GLU:HB2	1:D:359:ARG:HD2	1.96	0.47
1:C:73:ARG:HG3	1:C:85:LEU:HB3	1.97	0.47
1:D:214:TYR:CD1	1:D:217:MET:HE2	2.50	0.46
1:C:57:ILE:HG23	1:C:97:LEU:O	2.16	0.45
1:A:85:LEU:HD21	1:A:104:LEU:HD13	1.98	0.45
1:A:170:HIS:HA	1:A:173:LEU:HD12	1.99	0.44
1:C:121:PHE:O	1:C:125:LEU:HG	2.16	0.44
1:A:250:VAL:HA	1:A:332:PHE:CD1	2.53	0.44
1:D:170:HIS:HA	1:D:173:LEU:HD12	2.00	0.43
1:B:250:VAL:HA	1:B:332:PHE:CD1	2.53	0.43
1:C:250:VAL:HA	1:C:332:PHE:CD1	2.54	0.43
1:D:143:ILE:HB	1:D:161:ILE:HB	1.99	0.43
1:C:55:ILE:HB	1:C:97:LEU:HD23	2.01	0.43
1:C:170:HIS:HA	1:C:173:LEU:HD12	2.00	0.43
1:C:372:SER:HA	1:C:375:GLU:HB2	2.00	0.42
1:B:193:LYS:HD3	1:B:211:SER:HB3	2.01	0.42
1:D:193:LYS:HD3	1:D:211:SER:HB3	2.01	0.42
1:A:175:LEU:HD13	1:A:215:VAL:HG11	2.02	0.42
1:D:250:VAL:HA	1:D:332:PHE:CD1	2.55	0.42
1:A:193:LYS:HD3	1:A:211:SER:HB3	2.02	0.41
1:C:188:MET:HE3	1:C:271:LEU:HB3	2.02	0.41
1:C:193:LYS:HD3	1:C:211:SER:HB3	2.03	0.41
1:D:372:SER:HA	1:D:375:GLU:HB2	2.02	0.41
1:B:372:SER:HA	1:B:375:GLU:HB2	2.02	0.41
1:B:175:LEU:HD13	1:B:215:VAL:HG11	2.03	0.40
1:A:372:SER:HA	1:A:375:GLU:HB2	2.04	0.40

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	311/405 (77%)	303 (97%)	8 (3%)	0	100	100
1	B	302/405 (75%)	298 (99%)	4 (1%)	0	100	100
1	C	308/405 (76%)	303 (98%)	5 (2%)	0	100	100
1	D	312/405 (77%)	304 (97%)	8 (3%)	0	100	100
All	All	1233/1620 (76%)	1208 (98%)	25 (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	284/363 (78%)	273 (96%)	11 (4%)	28	62
1	B	279/363 (77%)	267 (96%)	12 (4%)	26	59
1	C	278/363 (77%)	265 (95%)	13 (5%)	23	57
1	D	282/363 (78%)	270 (96%)	12 (4%)	26	59
All	All	1123/1452 (77%)	1075 (96%)	48 (4%)	26	59

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	78	ARG

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Mol	Chain	Res	Type
1	A	82	ASP
1	A	91	LEU
1	A	100	SER
1	A	117	ILE
1	A	158	GLN
1	A	160	ASP
1	A	217	MET
1	A	263	GLN
1	A	271	LEU
1	B	46	LYS
1	B	57	ILE
1	B	91	LEU
1	B	100	SER
1	B	117	ILE
1	B	125	LEU
1	B	173	LEU
1	B	176	SER
1	B	205	TYR
1	B	263	GLN
1	B	271	LEU
1	B	362	ASN
1	C	46	LYS
1	C	57	ILE
1	C	82	ASP
1	C	91	LEU
1	C	97	LEU
1	C	100	SER
1	C	115	ASP
1	C	117	ILE
1	C	119	LEU
1	C	198	ARG
1	C	271	LEU
1	C	362	ASN
1	C	371	ASP
1	D	46	LYS
1	D	57	ILE
1	D	91	LEU
1	D	100	SER
1	D	126	ILE
1	D	149	THR
1	D	198	ARG
1	D	205	TYR

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Mol	Chain	Res	Type
1	D	263	GLN
1	D	271	LEU
1	D	312	HIS
1	D	362	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	GLN
1	A	165	ASN
1	A	200	GLN
1	A	362	ASN
1	B	120	GLN
1	B	171	ASN
1	B	200	GLN
1	C	120	GLN
1	C	165	ASN
1	C	170	HIS
1	C	171	ASN
1	D	120	GLN
1	D	165	ASN
1	D	170	HIS
1	D	200	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](#)

4 ligands are modelled in this entry.

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	ACT	D	501	-	3,3,3	0.78	0	3,3,3	1.17	0
2	ACT	B	501	-	3,3,3	1.02	0	3,3,3	1.16	0
2	ACT	A	501	-	3,3,3	1.04	0	3,3,3	1.34	0
2	ACT	C	501	-	3,3,3	0.88	0	3,3,3	0.97	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	319/405 (78%)	-0.11	2 (0%) 85 73	52, 82, 116, 144	0
1	B	312/405 (77%)	-0.39	2 (0%) 85 73	34, 56, 88, 119	0
1	C	316/405 (78%)	-0.16	3 (0%) 81 64	48, 73, 103, 122	0
1	D	320/405 (79%)	-0.17	5 (1%) 70 51	42, 70, 112, 144	0
All	All	1267/1620 (78%)	-0.21	12 (0%) 81 64	34, 69, 110, 144	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	GLY	3.5
1	D	311	GLU	3.1
1	D	156	SER	3.1
1	D	116	THR	2.5
1	B	308	SER	2.4
1	A	149	THR	2.4
1	D	115	ASP	2.3
1	C	379	ILE	2.2
1	B	158	GLN	2.2
1	C	156	SER	2.1
1	D	149	THR	2.0
1	C	42	LYS	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(Å ²)	Q<0.9
2	ACT	B	501	4/4	0.94	0.24	57,57,57,58	0
2	ACT	A	501	4/4	0.95	0.17	65,65,65,66	0
2	ACT	D	501	4/4	0.96	0.16	67,68,69,69	0
2	ACT	C	501	4/4	0.97	0.14	77,79,79,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.