



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:57 am GMT

PDB ID : 3N40
Title : Crystal structure of the immature envelope glycoprotein complex of Chikungunya virus.
Authors : Voss, J.; Vaney, M.C.; Duquerroy, S.; Rey, F.A.
Deposited on : 2010-05-21
Resolution : 2.17 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

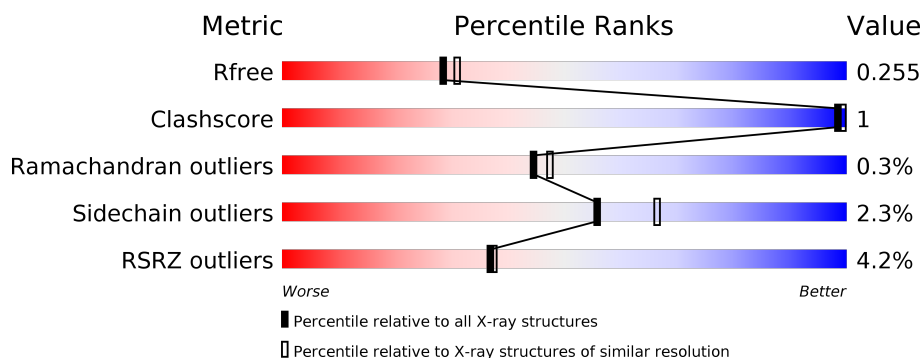
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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}	100719	5526 (2.20-2.16)
Clashscore	112137	6386 (2.20-2.16)
Ramachandran outliers	110173	6282 (2.20-2.16)
Sidechain outliers	110143	6282 (2.20-2.16)
RSRZ outliers	101464	5562 (2.20-2.16)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	P	401	<div> <div>7%</div> <div>95%</div> <div>.</div> </div>
2	F	393	<div> <div>2%</div> <div>96%</div> <div>.</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6669 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 P62 envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	401	Total	C	N	O	S	0	0	0
			3168	1973	568	598	29			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	64	GLU	ARG	ENGINEERED MUTATION	UNP Q1H8W5

- Molecule 2 is a protein called E1 envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	393	Total	C	N	O	S	0	1	0
			2995	1893	502	576	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	SEE REMARK 999	UNP Q1H8W5
F	0	GLY	-	SEE REMARK 999	UNP Q1H8W5

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

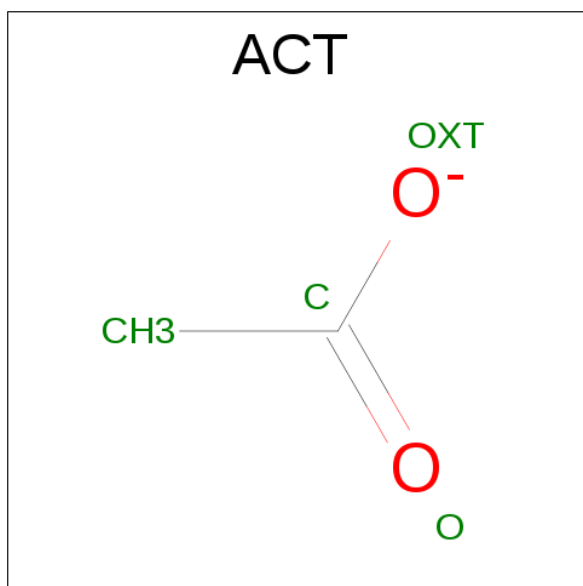
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	P	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	P	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

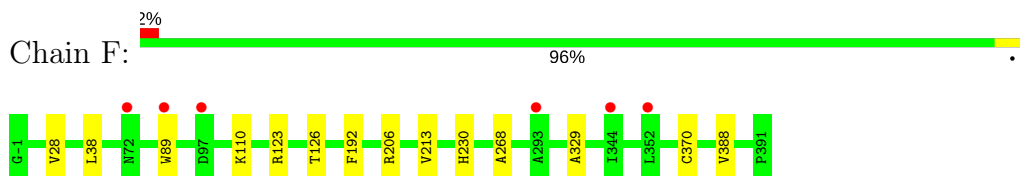
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	193	Total	O	0	0
			193	193		
7	F	223	Total	O	0	0
			223	223		

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- Molecule 1: P62 envelope glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.74Å 90.01Å 179.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.10 – 2.17 49.11 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.10-2.17) 99.3 (49.11-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.208 , 0.239 0.222 , 0.255	Depositor DCC
R_{free} test set	2582 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6669	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: NAG, NDG, 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	P	0.35	0/3253	0.58	0/4428
2	F	0.33	0/3072	0.57	0/4190
All	All	0.34	0/6325	0.58	0/8618

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

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	P	3168	0	3063	4	0
2	F	2995	0	2897	5	0
3	P	28	0	25	0	0
4	P	14	0	13	0	0
5	F	4	0	3	0	0
5	P	16	0	12	0	0
6	F	28	0	25	0	0
7	F	223	0	0	0	0
7	P	193	0	0	0	0
All	All	6669	0	6038	9	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 1.

All (9) 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:F:206:ARG:HH11	2:F:206:ARG:HG3	1.69	0.56
1:P:116:LEU:HD22	1:P:131:LEU:HD21	1.87	0.55
1:P:340:VAL:HG22	1:P:349:MET:HG2	1.93	0.51
2:F:38:LEU:HB2	2:F:268:ALA:HB3	1.93	0.50
2:F:110:LYS:HG3	2:F:213:VAL:HG11	1.93	0.49
2:F:28:VAL:HG23	2:F:329:ALA:HB1	1.96	0.46
1:P:312:LEU:HD13	1:P:315:ARG:HB2	1.99	0.44
2:F:192:PHE:CE1	2:F:206:ARG:HG2	2.52	0.44
1:P:106:THR:HB	1:P:200:ILE:HD11	2.04	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	P	399/401 (100%)	379 (95%)	19 (5%)	1 (0%)	44	47
2	F	392/393 (100%)	383 (98%)	8 (2%)	1 (0%)	44	47
All	All	791/794 (100%)	762 (96%)	27 (3%)	2 (0%)	44	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	126	THR
1	P	313	GLY

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	P	360/360 (100%)	349 (97%)	11 (3%)	45	54
2	F	329/328 (100%)	324 (98%)	5 (2%)	70	80
All	All	689/688 (100%)	673 (98%)	16 (2%)	56	66

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	9	LEU
1	P	64	GLU
1	P	137	HIS
1	P	222	GLN
1	P	247	GLN
1	P	271	ASN
1	P	287	ASP
1	P	312	LEU
1	P	329	THR
1	P	377	HIS
1	P	405	GLN
2	F	89	TRP
2	F	123	ARG
2	F	230	HIS
2	F	370	CYS
2	F	388	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

4 carbohydrates 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
6	NAG	F	1001	2,6	14,14,15	1.04	1 (7%)	15,19,21	0.92	0
6	NDG	F	1002	6	14,14,15	1.53	1 (7%)	15,19,21	1.23	1 (6%)
3	NAG	P	1001	1,3	14,14,15	1.20	1 (7%)	15,19,21	1.33	2 (13%)
3	NAG	P	1002	3	14,14,15	1.25	1 (7%)	15,19,21	0.83	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
6	NAG	F	1001	2,6	-	0/6/23/26	0/1/1/1
6	NDG	F	1002	6	-	0/6/23/26	0/1/1/1
3	NAG	P	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	1002	3	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	1001	NAG	C1-C2	2.70	1.56	1.52
3	P	1001	NAG	C1-C2	2.83	1.56	1.52
3	P	1002	NAG	C1-C2	3.29	1.57	1.52
6	F	1002	NDG	C1-C2	4.24	1.58	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1001	NAG	O4-C4-C3	-2.24	105.48	110.36
3	P	1001	NAG	C4-C3-C2	3.18	115.67	111.02
6	F	1002	NDG	C1-C2-N2	3.55	116.55	110.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

6 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$
5	ACT	F	392	-	1,3,3	1.86	0	0,3,3	0.00	-
5	ACT	P	1	-	1,3,3	1.90	0	0,3,3	0.00	-
5	ACT	P	2	-	1,3,3	2.10	1 (100%)	0,3,3	0.00	-
4	NAG	P	2001	1	14,14,15	1.31	1 (7%)	15,19,21	1.07	2 (13%)
5	ACT	P	3	-	1,3,3	1.92	0	0,3,3	0.00	-
5	ACT	P	406	-	1,3,3	1.89	0	0,3,3	0.00	-

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	ACT	F	392	-	-	0/0/0/0	0/0/0/0
5	ACT	P	1	-	-	0/0/0/0	0/0/0/0
5	ACT	P	2	-	-	0/0/0/0	0/0/0/0
4	NAG	P	2001	1	-	0/6/23/26	0/1/1/1
5	ACT	P	3	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ACT	P	406	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	2	ACT	CH3-C	2.10	1.51	1.48
4	P	2001	NAG	C1-C2	3.34	1.57	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	2001	NAG	C1-O5-C5	2.12	115.09	112.17
4	P	2001	NAG	C1-C2-N2	2.16	114.19	110.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	P	401/401 (100%)	0.58	27 (6%) 19 19	23, 38, 66, 80	0
2	F	393/393 (100%)	0.38	6 (1%) 74 74	22, 35, 58, 71	0
All	All	794/794 (100%)	0.48	33 (4%) 37 37	22, 36, 62, 80	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	283	ASN	7.0
1	P	249	SER	4.9
1	P	281	ILE	4.5
1	P	280	VAL	4.4
1	P	227	THR	4.1
1	P	226	ALA	4.1
1	P	282	ASN	3.9
1	P	312	LEU	3.7
1	P	310	ALA	3.1
1	P	311	GLU	3.1
2	F	293	ALA	3.1
1	P	377	HIS	3.0
1	P	352	TYR	2.9
1	P	206	HIS	2.9
2	F	89	TRP	2.9
1	P	247	GLN	2.8
1	P	88	GLU	2.8
1	P	271	ASN	2.7
1	P	314	ASP	2.6
2	F	352	LEU	2.6
1	P	270	SER	2.4
2	F	344	ILE	2.3
1	P	350	LEU	2.3
1	P	284	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	235	MET	2.2
1	P	273	GLY	2.2
1	P	267	CYS	2.1
2	F	97	ASP	2.1
1	P	224	THR	2.1
1	P	210	GLN	2.1
1	P	248	GLN	2.1
2	F	72	ASN	2.0
1	P	137	HIS	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	F	1001	14/15	0.95	0.14	-0.33	43,47,49,50	0
3	NAG	P	1001	14/15	0.72	0.21	-	62,66,68,68	0
6	NDG	F	1002	14/15	0.88	0.30	-	51,55,57,57	0
3	NAG	P	1002	14/15	0.79	0.23	-	68,72,75,75	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	ACT	F	392	4/4	0.91	0.16	1.42	44,44,44,45	0
5	ACT	P	406	4/4	0.84	0.19	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	ACT	P	1	4/4	0.93	0.16	-	54,54,54,54	0
5	ACT	P	3	4/4	0.94	0.16	-	54,54,54,55	0
4	NAG	P	2001	14/15	0.71	0.37	-	62,65,68,68	0
5	ACT	P	2	4/4	0.62	0.29	-	65,65,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.