



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2026 – 01:07 am BST

PDB ID : 9TB6 / pdb_00009tb6
Title : Crystal structure of the MpPYL1-HAB1 complex
Authors : Rivera-Moreno, M.; Infantes, L.; Albert, A.
Deposited on : 2025-11-19
Resolution : 2.39 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
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

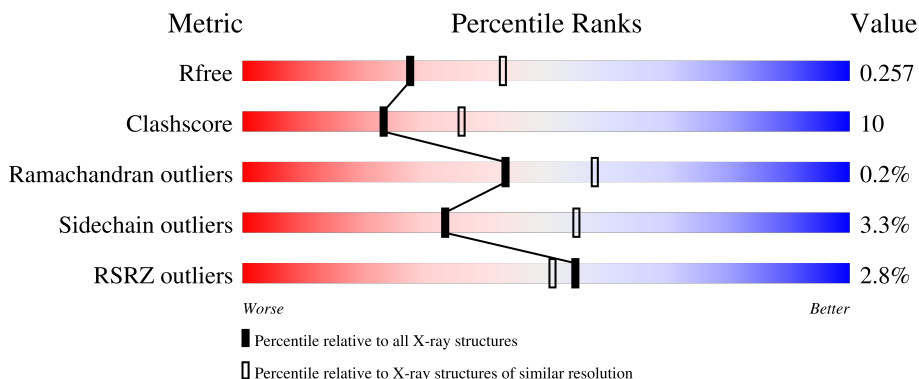
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	177	
2	B	332	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3990 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 PYL1 receptor from Marchantia polymorpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1395	866	254	271	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	initiating methionine	UNP A0A2R6X8C9

- Molecule 2 is a protein called Protein phosphatase 2C 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	329	Total	C	N	O	S	0	0	0
			2544	1598	454	473	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP Q9CAJ0
B	192	VAL	THR	conflict	UNP Q9CAJ0

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mn	0	0
			2	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		

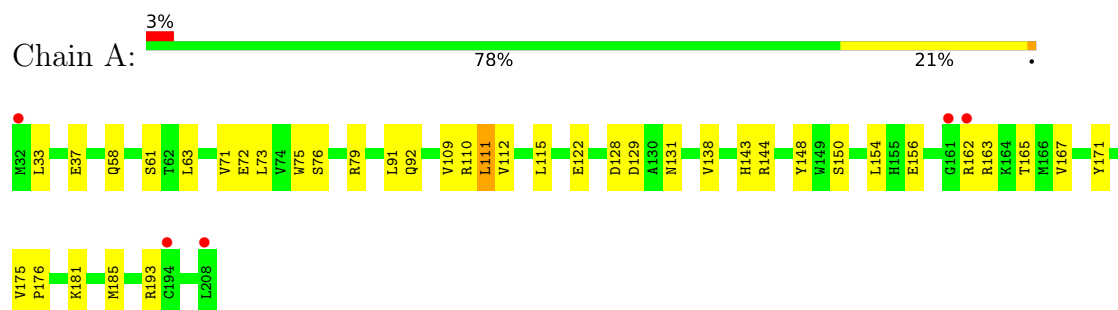
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total 19	O 19	0	0
5	B	28	Total 28	O 28	0	0

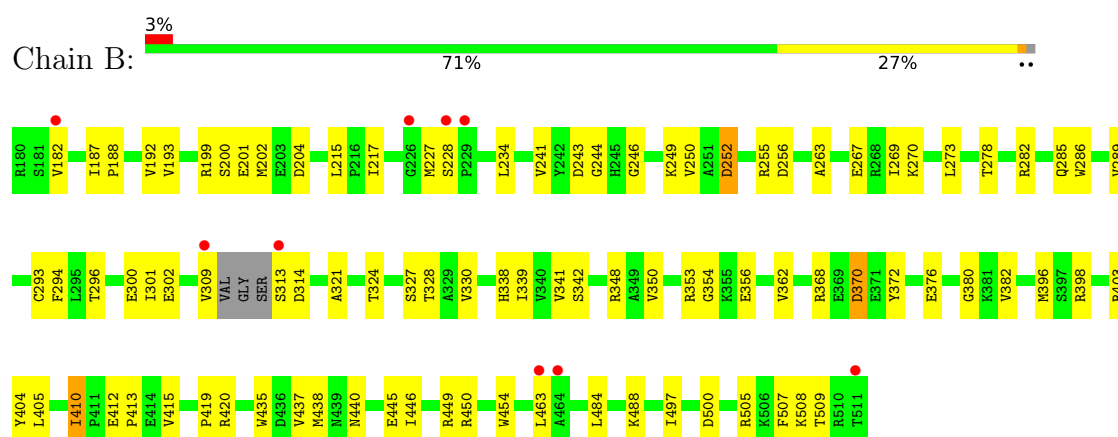
3 Residue-property plots [i](#)

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: PYL1 receptor from *Marchantia polymorpha*



- Molecule 2: Protein phosphatase 2C 16



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.12Å 71.52Å 103.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.85 – 2.39 58.85 – 2.39	Depositor EDS
% Data completeness (in resolution range)	64.0 (58.85-2.39) 64.0 (58.85-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.21.2-5419	Depositor
R, R_{free}	0.197 , 0.258 0.198 , 0.257	Depositor DCC
R_{free} test set	689 reflections (3.30%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3990	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% 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: MN, 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	0.40	0/1418	0.58	0/1922
2	B	0.42	0/2592	0.61	0/3496
All	All	0.41	0/4010	0.60	0/5418

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	A	1395	0	1373	30	0
2	B	2544	0	2526	57	0
3	B	2	0	0	0	0
4	B	2	0	0	1	0
5	A	19	0	0	0	0
5	B	28	0	0	2	0
All	All	3990	0	3899	81	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 10.

All (81) 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:110:ARG:HH21	2:B:200:SER:HB2	1.41	0.83
2:B:252:ASP:OD2	2:B:255:ARG:NH2	2.13	0.81
2:B:227:MET:SD	2:B:227:MET:N	2.55	0.78
2:B:215:LEU:HD22	2:B:286:TRP:HH2	1.52	0.74
1:A:61:SER:HB2	1:A:171:TYR:CE1	2.24	0.72
2:B:192:VAL:HG12	2:B:497:ILE:HG12	1.71	0.71
2:B:370:ASP:OD1	2:B:370:ASP:N	2.24	0.70
1:A:110:ARG:NH2	2:B:200:SER:HB2	2.06	0.70
1:A:175:VAL:HG21	1:A:181:LYS:HG2	1.73	0.70
2:B:410:ILE:HD12	2:B:412:GLU:HB2	1.76	0.66
1:A:72:GLU:H	1:A:72:GLU:CD	2.06	0.63
2:B:437:VAL:HG23	2:B:438:MET:HG3	1.80	0.63
1:A:91:LEU:HD22	1:A:109:VAL:HB	1.80	0.61
2:B:187:ILE:HD12	2:B:188:PRO:HD2	1.83	0.59
1:A:58:GLN:O	1:A:181:LYS:HE2	2.03	0.59
1:A:92:GLN:HE22	2:B:201:GLU:HG3	1.67	0.59
1:A:33:LEU:HD22	1:A:37:GLU:HB3	1.86	0.57
2:B:202:MET:HE3	2:B:204:ASP:O	2.06	0.56
1:A:75:TRP:HE3	1:A:154:LEU:HD12	1.71	0.56
2:B:199:ARG:HD2	5:B:719:HOH:O	2.07	0.55
2:B:217:ILE:HD12	2:B:234:LEU:HG	1.90	0.54
2:B:296:THR:O	2:B:300:GLU:HG3	2.07	0.54
1:A:92:GLN:HE22	2:B:201:GLU:CG	2.19	0.53
2:B:269:ILE:HD12	2:B:289:VAL:HG23	1.89	0.53
2:B:270:LYS:HA	2:B:273:LEU:HD12	1.92	0.52
1:A:110:ARG:HG2	1:A:110:ARG:HH11	1.74	0.52
2:B:278:THR:HG21	2:B:285:GLN:NE2	2.24	0.52
2:B:342:SER:HB2	2:B:415:VAL:HG22	1.91	0.52
2:B:398:ARG:HG2	2:B:410:ILE:HG13	1.92	0.52
1:A:128:ASP:OD1	1:A:131:ASN:N	2.35	0.51
1:A:112:VAL:HB	2:B:246:GLY:HA2	1.92	0.51
1:A:63:LEU:HD22	1:A:193:ARG:HG3	1.93	0.50
2:B:445:GLU:O	2:B:449:ARG:HG3	2.12	0.50
1:A:181:LYS:O	1:A:185:MET:HG3	2.13	0.49
2:B:362:VAL:HG12	2:B:368:ARG:HH11	1.78	0.49
2:B:454:TRP:HZ3	2:B:507:PHE:HE1	1.60	0.49
1:A:75:TRP:NE1	1:A:129:ASP:OD1	2.37	0.49
2:B:241:VAL:HB	2:B:330:VAL:HG13	1.94	0.48
1:A:71:VAL:HG22	1:A:165:THR:HG23	1.95	0.48
1:A:162:ARG:HH12	1:A:163:ARG:NH1	2.12	0.48
2:B:302:GLU:HG2	5:B:724:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:ILE:O	2:B:450:ARG:HG2	2.14	0.48
1:A:73:LEU:O	1:A:76:SER:OG	2.26	0.47
1:A:110:ARG:HG2	1:A:110:ARG:NH1	2.29	0.47
2:B:249:LYS:HG3	4:B:603:CL:CL	2.51	0.47
1:A:92:GLN:NE2	2:B:201:GLU:OE1	2.47	0.47
1:A:144:ARG:NH2	1:A:176:PRO:HB2	2.29	0.47
2:B:250:VAL:HG13	2:B:301:ILE:HD13	1.97	0.47
1:A:138:VAL:CG2	1:A:148:TYR:HB3	2.45	0.46
2:B:267:GLU:HA	2:B:270:LYS:HD2	1.98	0.46
1:A:138:VAL:HG11	1:A:143:HIS:CE1	2.51	0.46
2:B:339:ILE:HD12	2:B:420:ARG:HG2	1.98	0.46
2:B:341:VAL:O	2:B:415:VAL:HA	2.15	0.46
2:B:350:VAL:HG11	2:B:440:ASN:HB3	1.96	0.46
2:B:313:SER:OG	2:B:314:ASP:N	2.47	0.45
1:A:79:ARG:NH1	1:A:129:ASP:OD1	2.50	0.45
2:B:404:TYR:CE2	2:B:405:LEU:HG	2.51	0.45
2:B:182:VAL:HG13	2:B:217:ILE:HD11	1.99	0.45
2:B:263:ALA:O	2:B:267:GLU:HG3	2.16	0.45
2:B:321:ALA:O	2:B:403:ARG:NH2	2.47	0.44
2:B:372:TYR:CE1	2:B:382:VAL:HB	2.53	0.44
2:B:244:GLY:HA2	2:B:327:SER:HA	1.99	0.43
2:B:269:ILE:HG23	2:B:273:LEU:HD11	2.00	0.43
2:B:338:HIS:CD2	2:B:419:PRO:HA	2.54	0.43
1:A:79:ARG:NH1	1:A:129:ASP:OD2	2.51	0.43
1:A:111:LEU:HD23	1:A:115:LEU:HD12	2.01	0.43
2:B:376:GLU:HA	2:B:380:GLY:O	2.19	0.43
2:B:500:ASP:OD1	2:B:505:ARG:NH2	2.29	0.43
2:B:294:PHE:CD2	2:B:413:PRO:HB3	2.54	0.42
2:B:348:ARG:HB3	2:B:435:TRP:NE1	2.34	0.42
2:B:484:LEU:O	2:B:488:LYS:HG3	2.19	0.42
1:A:154:LEU:CD2	1:A:167:VAL:HG22	2.49	0.42
2:B:282:ARG:HE	2:B:282:ARG:HB2	1.71	0.42
2:B:241:VAL:HB	2:B:330:VAL:CG1	2.49	0.41
2:B:328:THR:HG22	2:B:396:MET:HE1	2.03	0.41
2:B:324:THR:HA	2:B:404:TYR:CE1	2.55	0.41
1:A:122:GLU:HG2	1:A:138:VAL:HG22	2.03	0.41
2:B:255:ARG:HG2	2:B:256:ASP:OD1	2.20	0.41
2:B:227:MET:H	2:B:227:MET:CE	2.34	0.40
2:B:356:GLU:O	2:B:356:GLU:HG2	2.21	0.40
2:B:243:ASP:O	2:B:328:THR:HG23	2.21	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	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
2	B	325/332 (98%)	307 (94%)	17 (5%)	1 (0%)	36	50
All	All	500/509 (98%)	474 (95%)	25 (5%)	1 (0%)	43	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	354	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	A	157/159 (99%)	154 (98%)	3 (2%)	50	71
2	B	272/278 (98%)	261 (96%)	11 (4%)	28	47
All	All	429/437 (98%)	415 (97%)	14 (3%)	33	55

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LEU
1	A	150	SER
1	A	156	GLU
2	B	193	VAL
2	B	228	SER

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Mol	Chain	Res	Type
2	B	252	ASP
2	B	293	CYS
2	B	309	VAL
2	B	353	ARG
2	B	370	ASP
2	B	410	ILE
2	B	463	LEU
2	B	508	LYS
2	B	509	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	92	GLN
1	A	131	ASN
1	A	143	HIS
1	A	205	GLN
2	B	343	ASN
2	B	377	ASN
2	B	458	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

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 [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	177/177 (100%)	0.20	5 (2%) 55 51	29, 38, 64, 87	0
2	B	329/332 (99%)	0.22	9 (2%) 56 52	25, 40, 58, 85	0
All	All	506/509 (99%)	0.21	14 (2%) 55 51	25, 40, 59, 87	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	MET	3.8
1	A	208	LEU	3.3
2	B	309	VAL	2.9
2	B	182	VAL	2.7
2	B	229	PRO	2.6
1	A	161	GLY	2.5
2	B	313	SER	2.4
2	B	463	LEU	2.4
2	B	464	ALA	2.2
1	A	162	ARG	2.2
2	B	228	SER	2.2
2	B	511	THR	2.2
2	B	226	GLY	2.1
1	A	194	CYS	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
4	CL	B	604	1/1	0.88	0.08	30,30,30,30	0
4	CL	B	603	1/1	0.89	0.09	60,60,60,60	0
3	MN	B	601	1/1	0.98	0.03	48,48,48,48	0
3	MN	B	602	1/1	0.99	0.05	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.