



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 12:42 AM JST

PDB ID : 7E5C
Title : Bacterial prolidase mutant D45W/L225Y/H226L/H343I
Authors : Yang, J.
Deposited on : 2021-02-18
Resolution : 2.22 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
Xtrriage (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

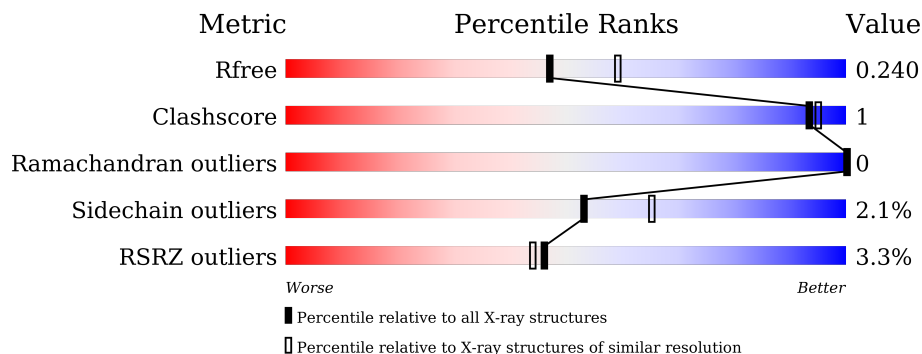
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	448	 94%
1	B	448	 93%
1	C	448	 93%
1	D	448	 93%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14635 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 Xaa-Pro dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	439	3569	2298	603	654	14	0	0	0
1	B	439	3569	2298	603	654	14	0	0	0
1	C	439	3569	2298	603	654	14	0	0	0
1	D	438	3560	2293	602	651	14	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	TRP	ASP	engineered mutation	UNP A0A1I7CHQ2
A	225	TYR	LEU	engineered mutation	UNP A0A1I7CHQ2
A	226	LEU	HIS	engineered mutation	UNP A0A1I7CHQ2
A	343	ILE	HIS	engineered mutation	UNP A0A1I7CHQ2
A	441	LEU	-	expression tag	UNP A0A1I7CHQ2
A	442	GLU	-	expression tag	UNP A0A1I7CHQ2
A	443	HIS	-	expression tag	UNP A0A1I7CHQ2
A	444	HIS	-	expression tag	UNP A0A1I7CHQ2
A	445	HIS	-	expression tag	UNP A0A1I7CHQ2
A	446	HIS	-	expression tag	UNP A0A1I7CHQ2
A	447	HIS	-	expression tag	UNP A0A1I7CHQ2
A	448	HIS	-	expression tag	UNP A0A1I7CHQ2
B	45	TRP	ASP	engineered mutation	UNP A0A1I7CHQ2
B	225	TYR	LEU	engineered mutation	UNP A0A1I7CHQ2
B	226	LEU	HIS	engineered mutation	UNP A0A1I7CHQ2
B	343	ILE	HIS	engineered mutation	UNP A0A1I7CHQ2
B	441	LEU	-	expression tag	UNP A0A1I7CHQ2
B	442	GLU	-	expression tag	UNP A0A1I7CHQ2
B	443	HIS	-	expression tag	UNP A0A1I7CHQ2
B	444	HIS	-	expression tag	UNP A0A1I7CHQ2
B	445	HIS	-	expression tag	UNP A0A1I7CHQ2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	446	HIS	-	expression tag	UNP A0A1I7CHQ2
B	447	HIS	-	expression tag	UNP A0A1I7CHQ2
B	448	HIS	-	expression tag	UNP A0A1I7CHQ2
C	45	TRP	ASP	engineered mutation	UNP A0A1I7CHQ2
C	225	TYR	LEU	engineered mutation	UNP A0A1I7CHQ2
C	226	LEU	HIS	engineered mutation	UNP A0A1I7CHQ2
C	343	ILE	HIS	engineered mutation	UNP A0A1I7CHQ2
C	441	LEU	-	expression tag	UNP A0A1I7CHQ2
C	442	GLU	-	expression tag	UNP A0A1I7CHQ2
C	443	HIS	-	expression tag	UNP A0A1I7CHQ2
C	444	HIS	-	expression tag	UNP A0A1I7CHQ2
C	445	HIS	-	expression tag	UNP A0A1I7CHQ2
C	446	HIS	-	expression tag	UNP A0A1I7CHQ2
C	447	HIS	-	expression tag	UNP A0A1I7CHQ2
C	448	HIS	-	expression tag	UNP A0A1I7CHQ2
D	45	TRP	ASP	engineered mutation	UNP A0A1I7CHQ2
D	225	TYR	LEU	engineered mutation	UNP A0A1I7CHQ2
D	226	LEU	HIS	engineered mutation	UNP A0A1I7CHQ2
D	343	ILE	HIS	engineered mutation	UNP A0A1I7CHQ2
D	441	LEU	-	expression tag	UNP A0A1I7CHQ2
D	442	GLU	-	expression tag	UNP A0A1I7CHQ2
D	443	HIS	-	expression tag	UNP A0A1I7CHQ2
D	444	HIS	-	expression tag	UNP A0A1I7CHQ2
D	445	HIS	-	expression tag	UNP A0A1I7CHQ2
D	446	HIS	-	expression tag	UNP A0A1I7CHQ2
D	447	HIS	-	expression tag	UNP A0A1I7CHQ2
D	448	HIS	-	expression tag	UNP A0A1I7CHQ2

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total 122	O 122	0	0
3	B	83	Total 83	O 83	0	0
3	C	61	Total 61	O 61	0	0
3	D	94	Total 94	O 94	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	182.97Å 182.97Å 372.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	67.45 – 2.22 67.36 – 2.22	Depositor EDS
% Data completeness (in resolution range)	93.9 (67.45-2.22) 93.9 (67.36-2.22)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.22Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.203 , 0.235 0.211 , 0.240	Depositor DCC
R_{free} test set	5564 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtrriage
Anisotropy	0.423	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14635	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: MN

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	0.66	0/3672	0.76	2/4987 (0.0%)
1	B	0.68	0/3672	0.74	1/4987 (0.0%)
1	C	0.74	0/3672	0.75	1/4987 (0.0%)
1	D	0.67	0/3662	0.75	0/4971
All	All	0.69	0/14678	0.75	4/19932 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	169	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	169	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	C	169	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	3569	0	3433	7	0
1	B	3569	0	3433	12	0
1	C	3569	0	3433	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3560	0	3427	11	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	122	0	0	1	0
3	B	83	0	0	2	2
3	C	61	0	0	0	2
3	D	94	0	0	0	0
All	All	14635	0	13726	38	2

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 (38) 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:C:129:ILE:HD12	1:C:150:MET:CE	1.94	0.98
1:B:394:LEU:O	1:B:397:THR:HG22	1.84	0.78
1:C:129:ILE:HD12	1:C:150:MET:HE1	1.70	0.73
1:C:129:ILE:HD12	1:C:150:MET:HE3	1.72	0.69
1:C:387:ILE:HG21	1:D:88:PHE:HB2	1.78	0.64
1:D:134:GLU:H	1:D:134:GLU:CD	2.01	0.64
1:B:20:ARG:O	1:B:24:GLU:HG2	1.98	0.64
1:C:58:ALA:HA	1:C:340:LEU:HD11	1.84	0.60
1:B:102:GLU:HG2	3:B:627:HOH:O	2.03	0.57
1:A:116:GLU:HG3	1:A:117:LYS:N	2.21	0.56
1:B:86:VAL:HG22	1:B:86:VAL:O	2.06	0.55
1:B:58:ALA:HA	1:B:340:LEU:HD11	1.88	0.55
1:D:87:ASP:OD2	1:D:89:TRP:CZ2	2.59	0.55
1:D:58:ALA:HA	1:D:340:LEU:HD11	1.90	0.53
1:A:116:GLU:CG	1:A:117:LYS:N	2.71	0.53
1:A:58:ALA:HA	1:A:340:LEU:HD11	1.90	0.53
1:A:79:LYS:HE2	1:A:107:GLU:HG3	1.93	0.51
1:D:93:PRO:O	1:D:94:ASP:HB3	2.13	0.49
1:A:397:THR:O	1:A:400:LYS:HE2	2.14	0.48
1:D:70:ILE:HG22	1:D:72:VAL:HG13	1.96	0.48
1:C:399:ASN:O	1:C:403:ILE:HD13	2.15	0.47
1:B:20:ARG:O	1:B:24:GLU:CG	2.64	0.46
1:D:150:MET:CE	1:D:150:MET:HA	2.46	0.45
1:D:147:GLU:N	1:D:148:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:TYR:CZ	1:C:85:PRO:HD3	2.52	0.45
1:D:93:PRO:O	1:D:94:ASP:CB	2.64	0.44
1:B:83:TYR:CE1	1:B:85:PRO:HD3	2.52	0.44
1:B:394:LEU:HD21	1:B:403:ILE:HD11	1.98	0.44
1:C:70:ILE:HG22	1:C:72:VAL:HG13	2.00	0.43
1:A:86:VAL:O	1:A:86:VAL:HG23	2.19	0.43
1:B:70:ILE:HG22	1:B:72:VAL:HG13	2.00	0.42
1:B:83:TYR:CZ	1:B:85:PRO:HD3	2.55	0.42
1:B:337:HIS:HD2	3:B:644:HOH:O	2.02	0.42
1:D:150:MET:HA	1:D:150:MET:HE2	2.01	0.42
1:D:226:LEU:O	1:D:228:THR:HG23	2.20	0.42
1:C:164:GLU:HG2	1:C:252:TYR:OH	2.21	0.41
1:B:397:THR:HG23	1:B:399:ASN:H	1.86	0.41
1:A:57:LYS:NZ	3:A:611:HOH:O	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:678:HOH:O	3:C:656:HOH:O[8_555]	2.13	0.07
3:B:623:HOH:O	3:C:659:HOH:O[8_555]	2.15	0.05

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	437/448 (98%)	431 (99%)	6 (1%)	0	100	100
1	B	437/448 (98%)	432 (99%)	5 (1%)	0	100	100
1	C	437/448 (98%)	434 (99%)	3 (1%)	0	100	100
1	D	434/448 (97%)	428 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1745/1792 (97%)	1725 (99%)	20 (1%)	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	378/387 (98%)	371 (98%)	7 (2%)	57	69
1	B	378/387 (98%)	370 (98%)	8 (2%)	53	65
1	C	378/387 (98%)	369 (98%)	9 (2%)	49	60
1	D	377/387 (97%)	370 (98%)	7 (2%)	57	69
All	All	1511/1548 (98%)	1480 (98%)	31 (2%)	53	65

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	97	ARG
1	A	117	LYS
1	A	142	SER
1	A	172	ASN
1	A	225	TYR
1	A	367	ARG
1	B	91	LYS
1	B	94	ASP
1	B	98	ASP
1	B	142	SER
1	B	172	ASN
1	B	225	TYR
1	B	301	GLN
1	B	398	ASP
1	C	86	VAL
1	C	121	TYR

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Mol	Chain	Res	Type
1	C	172	ASN
1	C	225	TYR
1	C	226	LEU
1	C	237	THR
1	C	315	LEU
1	C	388	ASP
1	C	428	ASP
1	D	86	VAL
1	D	97	ARG
1	D	116	GLU
1	D	134	GLU
1	D	172	ASN
1	D	225	TYR
1	D	342	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	ASN
1	D	151	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 8 ligands modelled in this entry, 8 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

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	439/448 (97%)	0.13	6 (1%) 75 73	37, 44, 70, 118	0
1	B	439/448 (97%)	-0.00	4 (0%) 84 83	33, 48, 72, 98	0
1	C	439/448 (97%)	0.32	36 (8%) 11 10	34, 51, 76, 112	0
1	D	438/448 (97%)	0.16	12 (2%) 54 52	38, 46, 72, 131	0
All	All	1755/1792 (97%)	0.15	58 (3%) 46 44	33, 47, 73, 131	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	89	TRP	5.6
1	A	94	ASP	5.5
1	C	92	VAL	5.3
1	B	89	TRP	4.9
1	D	92	VAL	4.7
1	D	93	PRO	4.7
1	C	402	PHE	4.5
1	C	93	PRO	4.2
1	C	398	ASP	3.9
1	A	89	TRP	3.8
1	C	225	TYR	3.7
1	C	121	TYR	3.7
1	D	88	PHE	3.5
1	C	410	GLU	3.4
1	C	311	ASN	3.4
1	C	395	ALA	3.3
1	C	394	LEU	3.3
1	C	399	ASN	3.2
1	C	361	GLU	3.1
1	D	90	HIS	3.0
1	C	355	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	321	VAL	2.8
1	B	121	TYR	2.8
1	C	314	LYS	2.8
1	C	396	GLN	2.8
1	C	406	GLU	2.8
1	C	367	ARG	2.8
1	D	89	TRP	2.8
1	D	94	ASP	2.8
1	D	236	HIS	2.7
1	C	403	ILE	2.7
1	D	225	TYR	2.7
1	A	361	GLU	2.6
1	C	365	PHE	2.5
1	D	226	LEU	2.4
1	C	90	HIS	2.4
1	C	312	ILE	2.4
1	D	398	ASP	2.3
1	A	124	ALA	2.3
1	C	362	GLY	2.3
1	A	121	TYR	2.3
1	C	316	PRO	2.3
1	D	361	GLU	2.3
1	C	305	GLN	2.2
1	D	365	PHE	2.2
1	C	308	SER	2.2
1	C	303	VAL	2.2
1	B	90	HIS	2.2
1	C	323	ARG	2.1
1	C	310	PHE	2.1
1	C	309	ASP	2.1
1	C	91	LYS	2.1
1	A	438	HIS	2.1
1	C	322	GLU	2.1
1	C	401	GLN	2.0
1	C	116	GLU	2.0
1	C	397	THR	2.0
1	B	97	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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(Å ²)	Q<0.9
2	MN	C	501	1/1	0.82	0.06	85,85,85,85	0
2	MN	C	502	1/1	0.90	0.04	85,85,85,85	0
2	MN	B	502	1/1	0.93	0.06	71,71,71,71	0
2	MN	A	502	1/1	0.93	0.09	71,71,71,71	0
2	MN	B	501	1/1	0.93	0.07	68,68,68,68	0
2	MN	D	501	1/1	0.95	0.09	63,63,63,63	0
2	MN	A	501	1/1	0.97	0.09	71,71,71,71	0
2	MN	D	502	1/1	0.97	0.10	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.