



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:34 AM UTC

PDB ID : 2V4B / pdb_00002v4b
Title : Crystal Structure of Human ADAMTS-1 catalytic Domain and Cysteine- Rich Domain (apo-form)
Authors : Gerhardt, S.; Hassall, G.; Hawtin, P.; McCall, E.; Flavell, L.; Minshull, C.; Hargreaves, D.; Ting, A.; Paupit, R.A.; Parker, A.E.; Abbott, W.M.
Deposited on : 2007-06-28
Resolution : 2.00 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

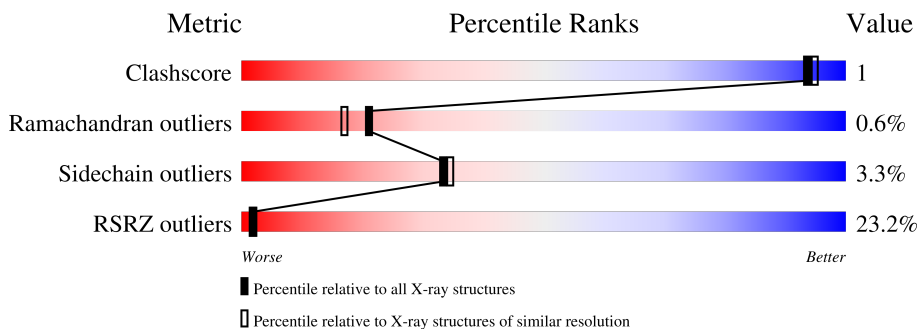
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	300	17% 88% 7%
1	B	300	26% 87% 7% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4556 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 ADAMTS-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2151	1337	374	415	25			
1	B	281	Total	C	N	O	S	0	0	0
			2164	1343	379	417	25			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cd	0	0
			2	2		
3	B	2	Total	Cd	0	0
			2	2		

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	Ni	0	0
			9	9		
4	B	5	Total	Ni	0	0
			5	5		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Mg 2	0	0
5	B	1	Total 1	Mg 1	0	0

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Na 2	0	0
6	B	2	Total 2	Na 2	0	0

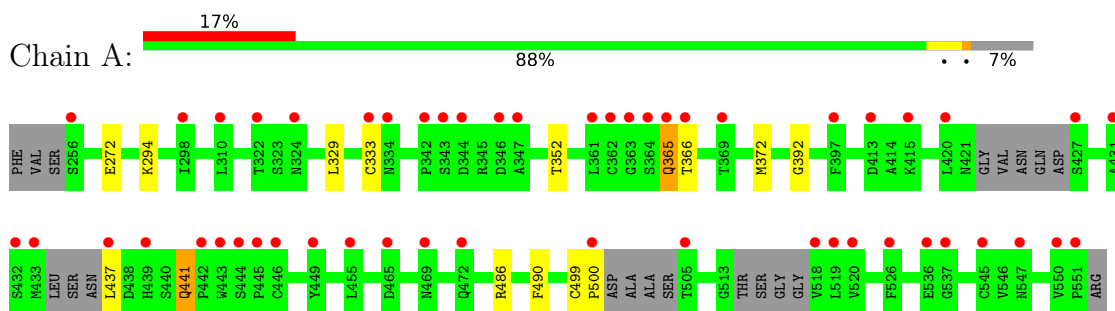
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	133	Total 133	O 133	0	0
7	B	81	Total 81	O 81	0	0

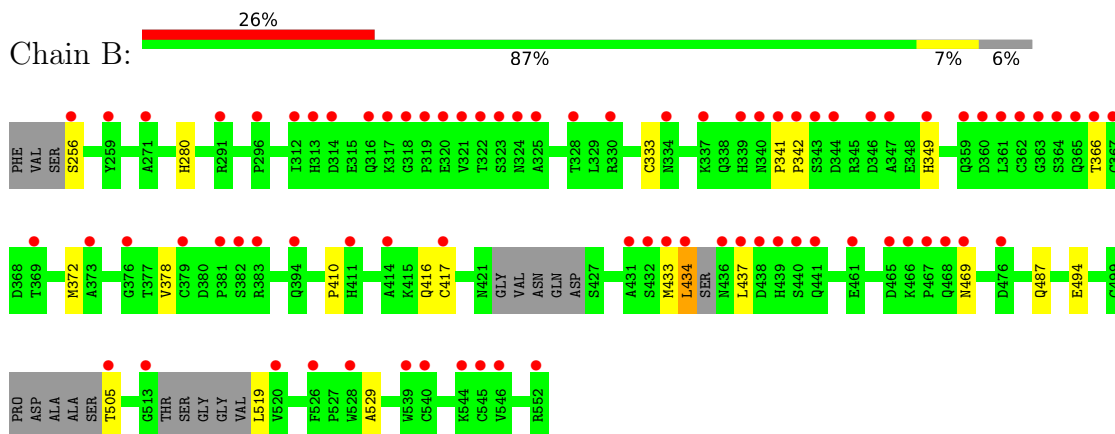
3 Residue-property plots [i](#)

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: ADAMTS-1



• Molecule 1: ADAMTS-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.58Å 64.40Å 113.52Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	40.26 – 2.00 40.26 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.26-2.00) 99.9 (40.26-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.220 , 0.263 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4556	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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: ZN, NA, MG, CD, NI

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	0/2202	0.79	0/2988
1	B	0.62	0/2214	0.80	1/3002 (0.0%)
All	All	0.64	0/4416	0.79	1/5990 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	VAL	N-CA-C	5.19	115.92	110.62

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	2151	0	2021	7	0
1	B	2164	0	2035	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	9	0	0	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	133	0	0	0	0
7	B	81	0	0	0	0
All	All	4556	0	4056	11	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 (11) 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:499:CYS:HA	1:A:500:PRO:C	2.02	0.85
1:B:487:GLN:HE22	1:B:529:ALA:H	1.45	0.64
1:B:341:PRO:O	1:B:349:HIS:HD2	1.91	0.54
1:A:441:GLN:HE21	1:A:441:GLN:HA	1.74	0.52
1:A:365:GLN:HG2	1:A:366:THR:H	1.78	0.47
1:A:392:GLY:HA2	1:A:490:PHE:HB3	1.97	0.47
1:A:329:LEU:HD22	1:A:372:MET:HG3	1.98	0.44
1:B:433:MET:O	1:B:434:LEU:C	2.60	0.44
1:A:499:CYS:CA	1:A:500:PRO:C	2.86	0.43
1:A:486:ARG:HD3	1:B:280:HIS:HB2	2.02	0.41
1:B:410:PRO:HG2	1:B:417:CYS:SG	2.60	0.41

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	270/300 (90%)	267 (99%)	2 (1%)	1 (0%)	30	27
1	B	271/300 (90%)	264 (97%)	5 (2%)	2 (1%)	18	14
All	All	541/600 (90%)	531 (98%)	7 (1%)	3 (1%)	21	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	366	THR
1	A	365	GLN
1	B	342	PRO

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	243/259 (94%)	237 (98%)	6 (2%)	42	45
1	B	244/259 (94%)	234 (96%)	10 (4%)	27	26
All	All	487/518 (94%)	471 (97%)	16 (3%)	33	34

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

Mol	Chain	Res	Type
1	A	272	GLU
1	A	294	LYS
1	A	333	CYS
1	A	352	THR
1	A	437	LEU
1	A	441	GLN
1	B	256	SER
1	B	333	CYS
1	B	372	MET
1	B	416	GLN
1	B	434	LEU
1	B	437	LEU
1	B	469	ASN

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Mol	Chain	Res	Type
1	B	494	GLU
1	B	505	THR
1	B	519	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	HIS
1	A	441	GLN
1	A	457	ASN
1	B	349	HIS
1	B	365	GLN
1	B	408	ASN
1	B	441	GLN
1	B	469	ASN
1	B	487	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](#)

Of 27 ligands modelled in this entry, 27 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 ⓘ

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	280/300 (93%)	1.23	51 (18%) 3 3	23, 35, 48, 57	0
1	B	281/300 (93%)	1.68	79 (28%) 1 1	26, 39, 56, 62	0
All	All	561/600 (93%)	1.45	130 (23%) 2 2	23, 37, 53, 62	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	434	LEU	6.0
1	B	344	ASP	5.4
1	A	344	ASP	4.7
1	A	551	PRO	4.5
1	B	439	HIS	4.4
1	B	367	CYS	4.4
1	B	316	GLN	4.2
1	B	364	SER	4.2
1	B	433	MET	4.2
1	B	546	VAL	4.2
1	B	321	VAL	4.1
1	B	365	GLN	4.0
1	B	431	ALA	3.9
1	B	363	GLY	3.8
1	A	363	GLY	3.7
1	B	318	GLY	3.7
1	B	526	PHE	3.7
1	B	505	THR	3.7
1	A	433	MET	3.6
1	B	366	THR	3.5
1	A	437	LEU	3.5
1	B	461	GLU	3.4
1	B	369	THR	3.4
1	A	439	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	373	ALA	3.4
1	A	520	VAL	3.4
1	B	436	ASN	3.3
1	A	500	PRO	3.3
1	B	513	GLY	3.2
1	B	323	SER	3.1
1	A	550	VAL	3.1
1	B	437	LEU	3.1
1	A	346	ASP	3.0
1	B	520	VAL	3.0
1	B	349	HIS	3.0
1	B	528	TRP	3.0
1	B	361	LEU	2.9
1	A	518	VAL	2.9
1	A	256	SER	2.9
1	B	362	CYS	2.9
1	B	312	ILE	2.9
1	B	465	ASP	2.9
1	B	314	ASP	2.8
1	B	411	HIS	2.9
1	B	440	SER	2.8
1	B	466	LYS	2.8
1	B	468	GLN	2.8
1	A	342	PRO	2.8
1	B	271	ALA	2.7
1	A	519	LEU	2.7
1	A	364	SER	2.7
1	A	536	GLU	2.7
1	A	505	THR	2.7
1	B	552	ARG	2.7
1	A	431	ALA	2.7
1	B	347	ALA	2.7
1	B	359	GLN	2.6
1	B	340	ASN	2.6
1	B	322	THR	2.6
1	B	346	ASP	2.6
1	B	259	TYR	2.6
1	B	441	GLN	2.6
1	A	413	ASP	2.6
1	B	339	HIS	2.6
1	A	334	ASN	2.6
1	A	427	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	365	GLN	2.5
1	A	472	GLN	2.5
1	A	333	CYS	2.5
1	B	317	LYS	2.5
1	B	324	ASN	2.5
1	B	256	SER	2.5
1	B	432	SER	2.5
1	B	379	CYS	2.5
1	B	469	ASN	2.5
1	B	394	GLN	2.5
1	A	420	LEU	2.5
1	B	414	ALA	2.5
1	A	310	LEU	2.5
1	A	455	LEU	2.5
1	A	547	ASN	2.5
1	A	449	TYR	2.4
1	A	432	SER	2.4
1	A	343	SER	2.4
1	B	328	THR	2.4
1	B	467	PRO	2.4
1	B	383	ARG	2.4
1	B	360	ASP	2.4
1	A	298	ILE	2.4
1	B	545	CYS	2.4
1	A	526	PHE	2.3
1	B	343	SER	2.3
1	B	313	HIS	2.3
1	A	444	SER	2.3
1	B	417	CYS	2.3
1	B	476	ASP	2.3
1	B	334	ASN	2.3
1	A	361	LEU	2.3
1	A	366	THR	2.2
1	A	469	ASN	2.2
1	A	545	CYS	2.2
1	B	325	ALA	2.2
1	B	337	LYS	2.2
1	B	342	PRO	2.2
1	B	376	GLY	2.2
1	A	324	ASN	2.2
1	A	369	THR	2.2
1	A	362	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	322	THR	2.2
1	B	296	PRO	2.1
1	B	320	GLU	2.1
1	A	442	PRO	2.1
1	A	537	GLY	2.1
1	B	291	ARG	2.1
1	B	438	ASP	2.1
1	B	381	PRO	2.1
1	A	347	ALA	2.1
1	B	382	SER	2.1
1	A	465	ASP	2.1
1	B	319	PRO	2.1
1	B	330	ARG	2.1
1	B	544	LYS	2.1
1	A	397	PHE	2.1
1	A	445	PRO	2.0
1	B	341	PRO	2.0
1	A	415	LYS	2.0
1	A	443	TRP	2.0
1	B	539	TRP	2.0
1	A	446	CYS	2.0
1	B	540	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($\text{\AA}^2$)	Q<0.9
5	MG	B	1558	1/1	0.88	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NA	A	1567	1/1	0.92	0.12	40,40,40,40	0
4	NI	B	1560	1/1	0.93	0.15	64,64,64,64	0
6	NA	B	1563	1/1	0.93	0.10	45,45,45,45	0
4	NI	A	1559	1/1	0.94	0.14	59,59,59,59	0
5	MG	A	1560	1/1	0.95	0.11	39,39,39,39	0
4	NI	A	1561	1/1	0.95	0.11	34,34,34,34	0
4	NI	A	1563	1/1	0.96	0.07	48,48,48,48	0
4	NI	A	1564	1/1	0.96	0.12	68,68,68,68	0
6	NA	B	1562	1/1	0.96	0.09	45,45,45,45	0
5	MG	A	1565	1/1	0.96	0.09	52,52,52,52	0
4	NI	B	1559	1/1	0.97	0.09	30,30,30,30	0
3	CD	B	1556	1/1	0.97	0.15	41,41,41,41	0
2	ZN	B	1553	1/1	0.98	0.08	26,26,26,26	0
4	NI	B	1561	1/1	0.98	0.06	44,44,44,44	0
4	NI	B	1557	1/1	0.98	0.09	29,29,29,29	0
3	CD	A	1554	1/1	0.98	0.10	35,35,35,35	0
4	NI	A	1557	1/1	0.99	0.06	28,28,28,28	0
4	NI	A	1558	1/1	0.99	0.04	37,37,37,37	0
2	ZN	A	1552	1/1	0.99	0.05	25,25,25,25	0
3	CD	B	1554	1/1	0.99	0.06	43,43,43,43	0
4	NI	A	1562	1/1	0.99	0.08	53,53,53,53	0
3	CD	A	1553	1/1	0.99	0.10	38,38,38,38	0
6	NA	A	1566	1/1	0.99	0.06	29,29,29,29	0
4	NI	A	1555	1/1	0.99	0.06	40,40,40,40	0
4	NI	B	1555	1/1	0.99	0.05	49,49,49,49	0
4	NI	A	1556	1/1	0.99	0.02	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.