



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:20 am BST

PDB ID : 5Z0T
Title : Thermoactinomyces vulgaris R-47 alpha-amylase I (TVA I) mutant
A357V/Q359N/Y360E (AQY/VNE)
Authors : Tonozuka, T.
Deposited on : 2017-12-21
Resolution : 1.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

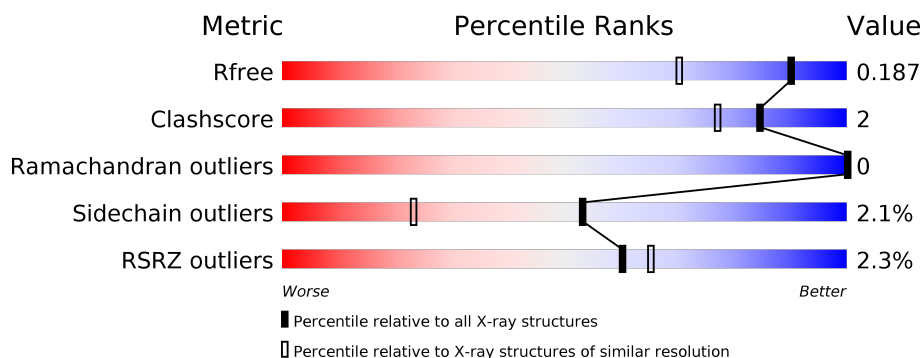
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 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	637	<div> <div>4%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	B	637	<div> <div>%</div> <div> <div></div> <div>95%</div> <div></div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12061 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 Neopullulanase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	637	Total	C	N	O	S	0	2	0
			5042	3193	842	997	10			
1	B	637	Total	C	N	O	S	0	3	0
			5045	3195	842	998	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	VAL	ALA	engineered mutation	UNP Q60053
A	359	ASN	GLN	engineered mutation	UNP Q60053
A	360	GLU	TYR	engineered mutation	UNP Q60053
B	357	VAL	ALA	engineered mutation	UNP Q60053
B	359	ASN	GLN	engineered mutation	UNP Q60053
B	360	GLU	TYR	engineered mutation	UNP Q60053

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		

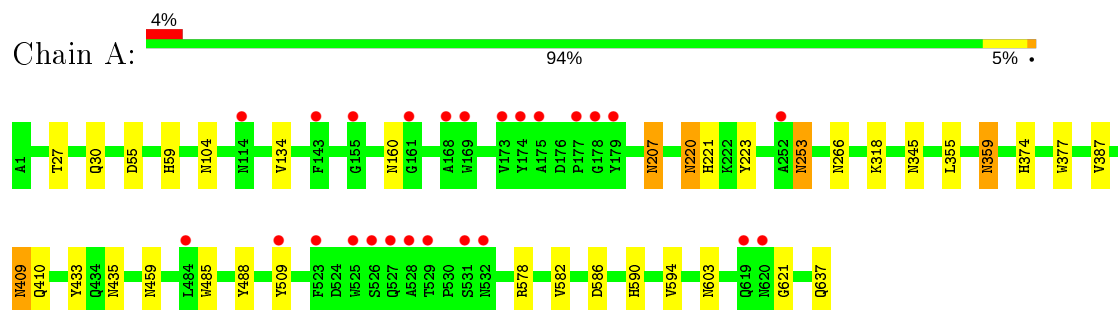
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	931	Total	O	0	0
			931	931		
4	B	1021	Total	O	0	0
			1021	1021		

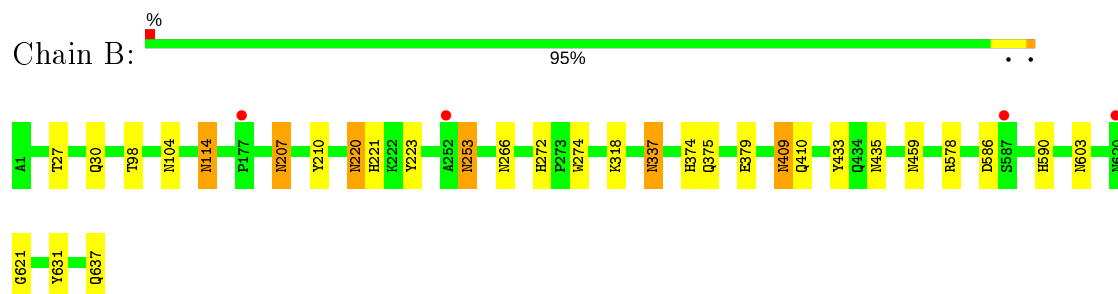
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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: Neopullulanase 1



• Molecule 1: Neopullulanase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.89Å 50.75Å 121.90Å 90.00° 103.91° 90.00°	Depositor
Resolution (Å)	46.91 – 1.50 23.45 – 1.50	Depositor EDS
% Data completeness (in resolution range)	89.4 (46.91-1.50) 89.4 (23.45-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.158 , 0.184 0.162 , 0.187	Depositor DCC
R_{free} test set	9022 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	9.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12061	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8094e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: CA, MPD

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	0.46	0/5204	0.66	0/7120
1	B	0.44	0/5210	0.66	0/7128
All	All	0.45	0/10414	0.66	0/14248

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	5042	0	4657	23	0
1	B	5045	0	4662	23	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	8	0	14	0	0
3	B	8	0	14	0	0
4	A	931	0	0	0	0
4	B	1021	0	0	0	0
All	All	12061	0	9347	44	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 (44) 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:B:578:ARG:HE	1:B:637:GLN:HE21	1.23	0.85
1:A:578:ARG:HE	1:A:637:GLN:HE21	1.30	0.80
1:B:603:ASN:HD21	1:B:621:GLY:H	1.40	0.70
1:A:27:THR:H	1:A:30:GLN:HE21	1.40	0.70
1:A:59:HIS:HD2	1:B:98:THR:O	1.75	0.69
1:A:266:ASN:HD21	1:A:318:LYS:HE2	1.60	0.66
1:B:207:ASN:H	1:B:207:ASN:HD22	1.46	0.64
1:A:207:ASN:H	1:A:207:ASN:HD22	1.46	0.62
1:A:485:TRP:HA	1:A:488:TYR:CD2	2.33	0.62
1:B:374:HIS:HD2	1:B:410:GLN:OE1	1.83	0.61
1:B:221:HIS:HD2	1:B:223:TYR:H	1.47	0.60
1:A:374:HIS:HD2	1:A:410:GLN:OE1	1.84	0.60
1:B:27:THR:H	1:B:30:GLN:HE21	1.48	0.60
1:A:221:HIS:HD2	1:A:223:TYR:H	1.53	0.56
1:A:603:ASN:HD21	1:A:621:GLY:H	1.53	0.55
1:A:409:ASN:HD21	1:A:410:GLN:HE21	1.53	0.55
1:B:578:ARG:HE	1:B:637:GLN:NE2	2.00	0.54
1:B:266:ASN:HD21	1:B:318:LYS:HE2	1.73	0.54
1:B:114:ASN:C	1:B:114:ASN:HD22	2.12	0.52
1:B:409:ASN:HD21	1:B:410:GLN:HE21	1.58	0.51
1:A:582:VAL:HG21	1:A:594:VAL:HG21	1.92	0.50
1:A:359:ASN:HD22	1:A:359:ASN:H	1.60	0.49
1:B:603:ASN:ND2	1:B:621:GLY:H	2.09	0.49
1:B:221:HIS:CD2	1:B:223:TYR:H	2.30	0.48
1:B:207:ASN:HD22	1:B:207:ASN:N	2.11	0.48
1:A:207:ASN:N	1:A:207:ASN:HD22	2.12	0.48
1:A:220:ASN:HD22	1:A:221:HIS:N	2.12	0.47
1:B:586:ASP:OD2	1:B:590:HIS:HE1	1.98	0.47
1:A:253:ASN:HD22	1:A:253:ASN:H	1.63	0.46
1:A:586:ASP:OD2	1:A:590:HIS:HE1	1.99	0.46
1:B:220:ASN:HD22	1:B:221:HIS:N	2.15	0.45
1:B:409:ASN:H	1:B:409:ASN:HD22	1.65	0.44
1:B:603:ASN:HD21	1:B:621:GLY:N	2.12	0.44
1:A:603:ASN:ND2	1:A:621:GLY:H	2.17	0.43
1:B:272:HIS:CE1	1:B:274:TRP:CD2	3.07	0.43
1:A:345:ASN:ND2	1:A:387:VAL:HG13	2.34	0.43
1:A:134:VAL:H	1:A:207:ASN:ND2	2.17	0.42
1:A:55:ASP:OD1	1:A:59:HIS:HE1	2.03	0.42
1:A:59:HIS:CD2	1:B:98:THR:O	2.64	0.42
1:B:253:ASN:H	1:B:253:ASN:HD22	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LEU:HD13	1:A:377:TRP:CZ3	2.56	0.41
1:B:375:GLN:NE2	1:B:379:GLU:OE2	2.53	0.41
1:B:337:ASN:HD22	1:B:337:ASN:H	1.68	0.40
1:A:221:HIS:CD2	1:A:223:TYR:H	2.35	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	637/637 (100%)	620 (97%)	17 (3%)	0	100	100
1	B	638/637 (100%)	619 (97%)	19 (3%)	0	100	100
All	All	1275/1274 (100%)	1239 (97%)	36 (3%)	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	543/541 (100%)	532 (98%)	11 (2%)	55	25
1	B	544/541 (101%)	532 (98%)	12 (2%)	52	22
All	All	1087/1082 (100%)	1064 (98%)	23 (2%)	53	23

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	160	ASN
1	A	207	ASN
1	A	220	ASN
1	A	253	ASN
1	A	359	ASN
1	A	409	ASN
1	A	433	TYR
1	A	435	ASN
1	A	459	ASN
1	A	509	TYR
1	B	104	ASN
1	B	114	ASN
1	B	207	ASN
1	B	210	TYR
1	B	220	ASN
1	B	253	ASN
1	B	337	ASN
1	B	409	ASN
1	B	433	TYR
1	B	435	ASN
1	B	459	ASN
1	B	631	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	30	GLN
1	A	56	ASN
1	A	59	HIS
1	A	68	ASN
1	A	104	ASN
1	A	123	ASN
1	A	160	ASN
1	A	195	GLN
1	A	207	ASN
1	A	220	ASN
1	A	221	HIS
1	A	226	GLN
1	A	253	ASN

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Mol	Chain	Res	Type
1	A	266	ASN
1	A	314	ASN
1	A	323	ASN
1	A	345	ASN
1	A	359	ASN
1	A	364	ASN
1	A	374	HIS
1	A	407	GLN
1	A	409	ASN
1	A	410	GLN
1	A	435	ASN
1	A	459	ASN
1	A	512	GLN
1	A	539	GLN
1	A	546	ASN
1	A	575	ASN
1	A	585	ASN
1	A	590	HIS
1	A	603	ASN
1	A	637	GLN
1	B	10	ASN
1	B	30	GLN
1	B	104	ASN
1	B	114	ASN
1	B	123	ASN
1	B	160	ASN
1	B	195	GLN
1	B	207	ASN
1	B	220	ASN
1	B	221	HIS
1	B	253	ASN
1	B	266	ASN
1	B	296	ASN
1	B	337	ASN
1	B	345	ASN
1	B	364	ASN
1	B	374	HIS
1	B	409	ASN
1	B	410	GLN
1	B	435	ASN
1	B	459	ASN
1	B	539	GLN

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Mol	Chain	Res	Type
1	B	546	ASN
1	B	585	ASN
1	B	590	HIS
1	B	593	ASN
1	B	603	ASN
1	B	614	HIS
1	B	637	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	MPD	A	704	-	7,7,7	0.30	0	9,10,10	0.44	0
3	MPD	B	704	-	7,7,7	0.30	0	9,10,10	0.42	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
3	MPD	A	704	-	-	0/5/5/5	-
3	MPD	B	704	-	-	0/5/5/5	-

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	637/637 (100%)	0.21	25 (3%) 39 44	7, 13, 23, 37	0
1	B	637/637 (100%)	-0.08	4 (0%) 89 91	7, 10, 16, 24	0
All	All	1274/1274 (100%)	0.06	29 (2%) 60 65	7, 11, 21, 37	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	LEU	5.4
1	A	169	TRP	3.3
1	A	525	TRP	3.2
1	A	529	THR	3.1
1	A	177	PRO	3.0
1	A	620	ASN	3.0
1	A	173	VAL	2.9
1	A	531	SER	2.9
1	A	619	GLN	2.8
1	A	509	TYR	2.8
1	A	175	ALA	2.7
1	B	252	ALA	2.7
1	A	527	GLN	2.6
1	A	143	PHE	2.5
1	A	178	GLY	2.5
1	A	523	PHE	2.4
1	A	114	ASN	2.4
1	A	179	TYR	2.4
1	A	168	ALA	2.3
1	A	528	ALA	2.3
1	A	161	GLY	2.3
1	B	177	PRO	2.2
1	A	532	ASN	2.2
1	B	587	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	155	GLY	2.1
1	A	174	TYR	2.1
1	B	620	ASN	2.1
1	A	526	SER	2.1
1	A	252	ALA	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 carbohydrates 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(\AA^2)	Q<0.9
3	MPD	A	704	8/8	0.83	0.19	27,29,31,32	0
3	MPD	B	704	8/8	0.87	0.16	19,21,25,26	0
2	CA	A	702	1/1	0.95	0.09	17,17,17,17	0
2	CA	A	703	1/1	0.98	0.04	15,15,15,15	0
2	CA	B	703	1/1	0.99	0.04	10,10,10,10	0
2	CA	B	701	1/1	1.00	0.04	8,8,8,8	0
2	CA	A	701	1/1	1.00	0.06	8,8,8,8	0
2	CA	B	702	1/1	1.00	0.04	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.