

wwPDB X-ray Structure Validation Summary Report (i)

Nov 20, 2023 – 04:58 PM JST

PDB ID : 7CWV	
Title : Crystal structure of Arabinose isomerase from hyper thermophilic ba	cterium
Thermotoga maritima (TMAI) wt	
Authors : Hoang, N.K.Q.; Dhanasingh, I.; Cao, T.P.; Sung, J.Y.; Shin, S.M.; Le	e, D.W.;
Lee, S.H.	
Deposited on : 2020-08-31	
Resolution : 3.53 Å(reported)	

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) 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	:	2.36
buster-report	:	1.1.7 (2018)
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 (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.53 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1028 (3.60-3.48)
Clashscore	141614	1109(3.60-3.48)
Ramachandran outliers	138981	1073 (3.60-3.48)
Sidechain outliers	138945	1074 (3.60-3.48)
RSRZ outliers	127900	1079 (3.62-3.46)

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 <=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	А	496	63%	33%	•••		
1	В	496	70%	27%	•		
1	С	496	% 60%	37%	•••		
1	D	496	67%	29%	•		
1	Е	496	3% 64%	33%	•		

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Mol	Chain	Length	Quality of chain		
1	F	496	63%	34%	•
1	G	496	2% 68%	28%	•
1	Н	496	% 68%	30%	•
1	Ι	496	^{2%} 67%	31%	
1	J	496	% 64%	33%	•
1	K	496	.% 66%	31%	•
1	L	496	^{2%} 72 %	27%	•



$7\mathrm{CWV}$

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 47714 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	401	Total	С	Ν	0	S	0	0	0
1	A	491	3943	2534	675	715	19	0	0	0
1	D	404	Total	С	Ν	0	S	0	0	0
	D	494	3973	2552	678	725	18	0	0	0
1	C	497	Total	С	Ν	0	S	0	0	0
	U	407	3930	2524	670	717	19	0	0	0
1	р	405	Total	С	Ν	0	S	0	0	0
	D	495	3981	2557	679	726	19	0	0	0
1	F	405	Total	С	Ν	Ο	S	0	0	0
	Ľ	495	3981	2557	679	726	19	0	0	0
1	Б	405	Total	С	Ν	0	S	0	0	0
	Г	495	3981	2557	679	726	19	0	0	0
1	C	405	Total	С	Ν	0	S	0	0	0
	G	495	3981	2557	679	726	19	0	0	0
1	ц	405	Total	С	Ν	0	S	0	0	0
1	11	495	3981	2557	679	726	19	0	0	0
1	т	405	Total	С	Ν	0	\mathbf{S}	0	0	0
1	1	495	3981	2557	679	726	19	0	0	0
1	т	405	Total	С	Ν	0	\mathbf{S}	0	0	0
1	J	495	3981	2557	679	726	19	0	0	0
1	K	405	Total	С	Ν	Ο	S	0	0	0
1	Γ	495	3981	2557	679	726	19	0	0	0
1	T	405	Total	С	Ν	0	S	0	0	0
1		490	3981	2557	679	726	19	0	0	0

• Molecule 1 is a protein called L-arabinose isomerase.

• Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Mn 1 1	0	0
2	В	1	Total Mn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	С	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	Е	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0
2	G	1	Total Mn 1 1	0	0
2	Н	1	Total Mn 1 1	0	0
2	Ι	1	Total Mn 1 1	0	0
2	J	1	Total Mn 1 1	0	0
2	K	1	Total Mn 1 1	0	0
2	L	1	Total Mn 1 1	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	С	1	Total 6	${ m C} { m 3}$	O 3	0	0



• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	5	Total O 5 5	0	0
4	В	1	Total O 1 1	0	0
4	С	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0
4	F	2	Total O 2 2	0	0
4	G	4	Total O 4 4	0	0
4	Н	1	Total O 1 1	0	0
4	Ι	1	Total O 1 1	0	0
4	J	2	Total O 2 2	0	0
4	К	2	Total O 2 2	0	0
4	L	1	Total O 1 1	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: L-arabinose isomerase





 \bullet Molecule 1: L-arabinose isomerase



• Molecule 1: L-arabinose isomerase

Chain E:

3%







Molecule 1: L-arabinose isomerase
 Chain G:
 68%
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• Molecule 1: L-arabinose isomerase



%

Chain J:







G324 T325

L281 P282 Q283 L284 P285 P285

V267 A268 V269 E483 L484 W491 G492 L493 L494 K495 ARG



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	85.97Å 109.43Å 153.85Å	Depositor
a, b, c, α , β , γ	98.14° 98.18° 89.97°	Depositor
Bosolution(A)	49.74 - 3.53	Depositor
Resolution (A)	49.70 - 3.53	EDS
% Data completeness	91.6 (49.74-3.53)	Depositor
(in resolution range)	91.6(49.70-3.53)	EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.30 (at 3.48 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
P. P.	0.222 , 0.332	Depositor
n, n_{free}	0.218 , 0.321	DCC
R_{free} test set	3146 reflections $(5.07%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	88.6	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.26, 65.4	EDS
L-test for $twinning^2$	$ < L >=0.42, < L^2>=0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	47714	wwPDB-VP
Average B, all atoms $(Å^2)$	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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, GOL

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	А	0.68	0/4036	0.82	0/5459	
1	В	0.67	0/4068	0.79	0/5505	
1	С	0.67	0/4023	0.81	0/5442	
1	D	0.68	0/4076	0.81	0/5515	
1	Ε	0.68	0/4076	0.80	0/5515	
1	F	0.67	0/4076	0.81	0/5515	
1	G	0.67	0/4076	0.82	0/5515	
1	Н	0.67	0/4076	0.80	0/5515	
1	Ι	0.67	0/4076	0.80	0/5515	
1	J	0.67	0/4076	0.79	0/5515	
1	Κ	0.67	0/4076	0.79	0/5515	
1	L	0.67	0/4076	0.79	0/5515	
All	All	0.67	0/48811	0.80	0/66041	

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 (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	А	3943	0	3971	125	0

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7	0	XX 7	V
1	U	vv	V

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	3973	0	3985	93	0
1	С	3930	0	3938	136	0
1	D	3981	0	3997	109	0
1	Е	3981	0	3997	121	0
1	F	3981	0	3997	118	0
1	G	3981	0	3997	114	0
1	Н	3981	0	3997	101	0
1	Ι	3981	0	3997	95	0
1	J	3981	0	3997	111	0
1	Κ	3981	0	3997	101	0
1	L	3981	0	3997	85	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	Е	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	Н	1	0	0	0	0
2	Ι	1	0	0	0	0
2	J	1	0	0	0	0
2	Κ	1	0	0	0	0
2	L	1	0	0	0	0
3	С	6	0	8	0	0
4	А	5	0	0	1	0
4	В	1	0	0	0	0
4	С	1	0	0	0	0
4	D	1	0	0	0	0
4	F	2	0	0	0	0
4	G	4	0	0	0	0
4	Н	1	0	0	0	0
4	Ι	1	0	0	0	0
4	J	2	0	0	0	0
4	Κ	2	0	0	0	0
4	L	1	0	0	0	0
All	All	47714	0	47875	1201	0

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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 13.

The worst 5 of 1201 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:I:162:LYS:HD2	1:I:455:GLU:HG2	1.57	0.87
1:J:403:ASN:HD21	1:J:426:PRO:HB3	1.42	0.84
1:C:180:ARG:NH2	1:C:184:ASN:OD1	2.12	0.83
1:L:278:LEU:O	1:L:371:LYS:NZ	2.11	0.83
1:E:145:LYS:HD3	1:E:459:ASP:OD1	1.81	0.80

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	Pe	erc	$\mathbf{entiles}$
1	А	487/496~(98%)	412 (85%)	67 (14%)	8 (2%)		9	46
1	В	492/496~(99%)	433 (88%)	48 (10%)	11 (2%)		6	39
1	С	483/496~(97%)	426 (88%)	46 (10%)	11 (2%)		6	38
1	D	493/496~(99%)	434 (88%)	44 (9%)	15 (3%)		4	33
1	Е	493/496~(99%)	430 (87%)	49 (10%)	14 (3%)		5	34
1	F	493/496~(99%)	428 (87%)	53 (11%)	12 (2%)		6	37
1	G	493/496~(99%)	427 (87%)	56 (11%)	10 (2%)		7	42
1	Н	493/496~(99%)	428 (87%)	55 (11%)	10 (2%)		7	42
1	Ι	493/496~(99%)	426 (86%)	54 (11%)	13 (3%)		5	35
1	J	493/496~(99%)	426 (86%)	56 (11%)	11 (2%)		6	39
1	K	493/496~(99%)	432 (88%)	50 (10%)	11 (2%)		6	39
1	L	493/496~(99%)	439 (89%)	45 (9%)	9 (2%)		8	43
All	All	5899/5952 (99%)	5141 (87%)	623 (11%)	135 (2%)		6	38

 $5~{\rm of}~135$ Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	323	GLY
	<i>a</i>	1	

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		1	1 0
Mol	Chain	\mathbf{Res}	Type
1	В	323	GLY
1	С	238	ILE
1	D	242	ASP
1	D	323	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	421/426~(99%)	397~(94%)	24 (6%)	20 55		
1	В	424/426~(100%)	407~(96%)	17 (4%)	31 65		
1	С	420/426~(99%)	399~(95%)	21 (5%)	24 59		
1	D	425/426~(100%)	406 (96%)	19 (4%)	27 62		
1	Ε	425/426~(100%)	405~(95%)	20 (5%)	26 61		
1	F	425/426~(100%)	397~(93%)	28 (7%)	16 50		
1	G	425/426~(100%)	397~(93%)	28 (7%)	16 50		
1	Н	425/426~(100%)	401 (94%)	24 (6%)	21 55		
1	Ι	425/426~(100%)	409 (96%)	16 (4%)	33 66		
1	J	425/426~(100%)	400 (94%)	25~(6%)	19 54		
1	Κ	425/426~(100%)	401 (94%)	24 (6%)	21 55		
1	L	425/426~(100%)	405 (95%)	20 (5%)	26 61		
All	All	5090/5112~(100%)	4824 (95%)	266 (5%)	23 58		

5 of 266 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Κ	219	LYS
1	Κ	373	ASP
1	L	331	TYR
1	Е	331	TYR
1	Е	274	THR



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	J	177	GLN
1	Κ	133	HIS
1	J	403	ASN
1	Κ	137	HIS
1	D	382	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 12 are monoatomic - leaving 1 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).

Mal	Tuno	Chain	Dog	Link	B	ond leng	gths	E	Bond ang	gles
WIOI	Type	Ullalli	nam nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	GOL	С	501	-	$5,\!5,\!5$	0.18	0	$5,\!5,\!5$	0.43	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	GOL	С	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	501	GOL	O1-C1-C2-O2
3	С	501	GOL	O1-C1-C2-C3

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, 95^{th} 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		>2	$OWAB(Å^2)$	Q<0.9
1	А	491/496~(98%)	-0.48	2(0%)	92	87	56, 102, 159, 278	0
1	В	494/496~(99%)	-0.34	5 (1%)	82	71	70, 113, 180, 228	0
1	С	487/496~(98%)	-0.36	3 (0%)	89	81	65, 108, 171, 216	0
1	D	495/496~(99%)	-0.30	7 (1%)	75	62	64, 112, 191, 271	0
1	Е	495/496~(99%)	-0.34	13 (2%)	56	42	60, 111, 179, 213	0
1	F	495/496~(99%)	-0.48	2(0%)	92	87	49, 102, 158, 222	0
1	G	495/496~(99%)	-0.31	8 (1%)	72	59	49, 105, 199, 283	0
1	Н	495/496~(99%)	-0.37	6 (1%)	79	67	64, 114, 171, 207	0
1	Ι	495/496~(99%)	-0.24	10 (2%)	65	52	68, 118, 184, 296	0
1	J	495/496~(99%)	-0.29	4 (0%)	86	75	68, 115, 184, 241	0
1	K	495/496~(99%)	-0.35	3 (0%)	89	81	67, 115, 188, 236	0
1	L	495/496~(99%)	-0.23	9 (1%)	68	54	67, 121, 184, 243	0
All	All	5927/5952~(99%)	-0.34	72 (1%)	79	67	49, 111, 181, 296	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ι	240	PRO	12.3
1	Ι	239	MET	6.2
1	G	240	PRO	5.6
1	Ι	418	PRO	5.0
1	L	380	ASP	4.3

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 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, 95^{th} 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	$B-factors(A^2)$	Q<0.9
2	MN	D	501	1/1	0.71	0.17	135,135,135,135	0
2	MN	Ι	501	1/1	0.88	0.08	112,112,112,112	0
2	MN	J	501	1/1	0.89	0.10	115,115,115,115	0
3	GOL	С	501	6/6	0.92	0.21	76,89,94,107	0
2	MN	Е	501	1/1	0.93	0.06	115,115,115,115	0
2	MN	Н	501	1/1	0.94	0.08	109,109,109,109	0
2	MN	G	501	1/1	0.94	0.10	99,99,99,99	0
2	MN	В	501	1/1	0.95	0.09	112,112,112,112	0
2	MN	K	501	1/1	0.96	0.12	117,117,117,117	0
2	MN	F	501	1/1	0.96	0.07	84,84,84,84	0
2	MN	L	501	1/1	0.98	0.04	85,85,85,85	0
2	MN	С	502	1/1	0.99	0.08	112,112,112,112	0
2	MN	A	501	1/1	1.00	0.06	84,84,84,84	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

















































6.5 Other polymers (i)

There are no such residues in this entry.

