

wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2024 - 10:03 PM EST

PDB ID	:	3VK4
Title	:	Crystal Structure of L-Methionine gamma-Lyase from Pseudomonas putida
		C116H Mutant complexed with L-homocysteine
Authors	:	Fukumoto, M.; Kudou, D.; Murano, S.; Shiba, T.; Sato, D.; Tamura, T.;
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Deposited on	:	2011-11-07
Resolution	:	2.61 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 (1)) 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
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 2.61 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	3797 (2.64-2.60)		
Clashscore	141614	4168 (2.64-2.60)		
Ramachandran outliers	138981	4093 (2.64-2.60)		
Sidechain outliers	138945	4093 (2.64-2.60)		
RSRZ outliers	127900	3731 (2.64-2.60)		

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	398	<mark>6%</mark> 73%	21%	5% •
1	В	398	7%	19%	
1	С	398	5%	22%	5% •
1	D	398	6% 69%	24%	5% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



Mol	Type	Chain	\mathbf{Res}	Chirality	Geometry	Clashes	Electron density
2	HCS	А	501	-	-	Х	Х
2	HCS	С	501	-	-	Х	Х
2	HCS	D	501	-	-	Х	-



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12018 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		Atoms				ZeroOcc	AltConf	Trace	
1	Δ	202	Total	С	Ν	0	Р	\mathbf{S}	0	0	0
1	A	392	2970	1874	525	554	1	16	0	0	0
1	В	306	Total	С	Ν	0	Р	S	0	0	0
1	D	390	2997	1889	531	560	1	16	0	0	0
1	C	202	Total	С	Ν	0	Р	S	0	0	0
1		392	2970	1874	525	554	1	16			
1	1 D	202	Total	С	Ν	0	Р	S	0	0	0
	392	2970	1874	525	554	1	16	0	0	U	

• Molecule 1 is a protein called Methionine gamma-lyase.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	116	HIS	CYS	engineered mutation	UNP P13254
В	116	HIS	CYS	engineered mutation	UNP P13254
С	116	HIS	CYS	engineered mutation	UNP P13254
D	116	HIS	CYS	engineered mutation	UNP P13254

• Molecule 2 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (three-letter code: HCS) (formula: $C_4H_9NO_2S$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	Λ	1	Total	С	Ν	0	S	0	0
	Л	I	8	4	1	2	1	0	0
9	В	1	Total	С	Ν	0	\mathbf{S}	0	0
	D	I	8	4	1	2	1	0	0
0	С	1	Total	С	Ν	Ο	S	0	0
	U	L	8	4	1	2	1	0	0
0	Л	1	Total	С	Ν	0	S	0	0
	D	L	8	4	1	2	1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	16	Total O 16 16	0	0
3	В	25	Total O 25 25	0	0
3	С	18	Total O 18 18	0	0
3	D	20	TotalO2020	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: Methionine gamma-lyase

A344 X211 L100 E345 S214 U107 F346 S214 U107 A356 S214 U107 A356 L230 L110 A356 L230 L114 A357 L336 L114 A357 L336 L114 A357 L336 L1416 A357 L336 L144 A358 L344 L144 A359 L344 L144 L366 L366 L144 L367 L364 L146 A393 L365 L144 L364 A345 L146 L364 A345 L146 L364 A345 L146 L364 A345 L146 L364 L365 L143 L364 L366 L146 L364 L366 L146 L364 L366 L146 L364 L366 L146

• Molecule 1: Methionine gamma-lyase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	153.49Å 153.49 Å 80.67 Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	29.28 - 2.61	Depositor
Resolution (A)	29.28 - 2.61	EDS
% Data completeness	98.2 (29.28-2.61)	Depositor
(in resolution range)	98.2 (29.28-2.61)	EDS
R_{merge}	0.15	Depositor
R _{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	$3.39 (at 2.61 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
D D	0.191 , 0.253	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.190 , 0.251	DCC
R_{free} test set	2901 reflections $(5.05%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	29.1	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36, 35.2	EDS
L-test for twinning ²	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12018	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.80% 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: LLP, HCS

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).

Mal	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.75	0/3010	0.81	1/4086~(0.0%)	
1	В	0.78	0/3037	0.81	1/4121~(0.0%)	
1	С	0.77	0/3010	0.85	6/4086~(0.1%)	
1	D	0.73	0/3010	0.79	1/4086~(0.0%)	
All	All	0.76	0/12067	0.82	9/16379~(0.1%)	

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	73	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	D	268	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	В	230	LEU	CA-CB-CG	5.72	128.46	115.30
1	А	233	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	С	387	LEU	CA-CB-CG	5.43	127.79	115.30

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	А	2970	0	2927	81	0
1	В	2997	0	2954	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	2970	0	2927	88	0
1	D	2970	0	2926	88	0
2	А	8	0	8	5	0
2	В	8	0	8	3	0
2	С	8	0	8	5	0
2	D	8	0	8	8	0
3	А	16	0	0	1	0
3	В	25	0	0	2	0
3	С	18	0	0	1	0
3	D	20	0	0	6	0
All	All	12018	0	11766	298	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 298 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:322:ILE:HG22	1:B:371:GLU:HB3	1.20	1.14
1:A:219:ILE:HD11	1:A:254:LEU:HD23	1.12	1.10
1:C:114:TYR:HE1	2:C:501:HCS:HB2	1.20	1.03
1:B:340:SER:HA	2:B:501:HCS:HB2	1.45	0.98
1:C:114:TYR:CE1	2:C:501:HCS:HB2	2.00	0.96

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	Analysed Favoured Allowed		Outliers	Percentiles
1	А	389/398~(98%)	369~(95%)	16 (4%)	4 (1%)	15 30
1	В	393/398~(99%)	365~(93%)	26 (7%)	2~(0%)	29 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percent	tiles			
1	С	389/398~(98%)	372 (96%)	15 (4%)	2~(0%)	29	50			
1	D	389/398~(98%)	361~(93%)	18 (5%)	10 (3%)	5 8	8			
All	All	1560/1592~(98%)	1467 (94%)	75~(5%)	18 (1%)	13	25			

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5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	55	ALA
1	А	340	SER
1	D	58	PHE
1	D	340	SER
1	А	322	ILE

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	А	301/306~(98%)	265~(88%)	36 (12%)	5 8
1	В	304/306~(99%)	270~(89%)	34 (11%)	6 10
1	С	301/306~(98%)	261~(87%)	40 (13%)	4 6
1	D	301/306~(98%)	270~(90%)	31 (10%)	7 12
All	All	1207/1224~(99%)	1066 (88%)	141 (12%)	5 9

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	99	THR
1	D	178	LYS
1	D	304	ARG
1	В	163	ASN
1	В	153	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:



Mol	Chain	Res	Type
1	С	207	HIS
1	D	207	HIS
1	С	237	GLN
1	D	57	HIS
1	D	263	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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 Tuno	Chain	Chain	Chain	Dog	Tipk	Bond lengths			Bond angles		
	Type	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
1	LLP	С	211	1	23,24,25	2.11	4 (17%)	25,32,34	1.83	5 (20%)	
1	LLP	А	211	1	23,24,25	2.28	5 (21%)	25,32,34	1.58	3 (12%)	
1	LLP	В	211	1	23,24,25	2.50	6 (26%)	25,32,34	1.77	6 (24%)	
1	LLP	D	211	1	23,24,25	2.36	4 (17%)	25,32,34	1.83	5 (20%)	

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
1	LLP	С	211	1	-	$\frac{5/16/17/19}{}$	0/1/1/1
1	LLP	А	211	1	-	4/16/17/19	0/1/1/1
1	LLP	В	211	1	-	6/16/17/19	0/1/1/1
1	LLP	D	211	1	-	5/16/17/19	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	D	211	LLP	C4'-NZ	6.96	1.50	1.27
1	В	211	LLP	C4'-NZ	6.69	1.49	1.27
1	А	211	LLP	C4'-NZ	6.41	1.48	1.27
1	В	211	LLP	C2'-C2	-6.34	1.39	1.50
1	С	211	LLP	C4'-NZ	6.10	1.47	1.27

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	С	211	LLP	C4-C3-C2	5.72	123.73	120.19
1	D	211	LLP	C4-C3-C2	5.63	123.67	120.19
1	А	211	LLP	C4-C3-C2	4.53	122.99	120.19
1	В	211	LLP	C4-C3-C2	4.15	122.76	120.19
1	В	211	LLP	C4-C4'-NZ	-3.37	108.82	124.31

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	211	LLP	O-C-CA-CB
1	В	211	LLP	O-C-CA-CB
1	С	211	LLP	N-CA-CB-CG
1	С	211	LLP	O-C-CA-CB
1	D	211	LLP	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	211	LLP	2	0
1	В	211	LLP	1	0
1	D	211	LLP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.



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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 True		Chain	Dog	Link	Bond lengths			Bond angles		
IVIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	HCS	В	501	-	6,7,7	0.85	0	7,8,8	1.91	1 (14%)
2	HCS	А	501	-	6,7,7	0.89	0	7,8,8	2.40	2 (28%)
2	HCS	D	501	-	6,7,7	0.85	0	7,8,8	1.33	1 (14%)
2	HCS	С	501	-	6,7,7	0.85	0	7,8,8	2.10	2 (28%)

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
2	HCS	В	501	-	-	7/7/7/7	-
2	HCS	А	501	-	-	5/7/7/7	-
2	HCS	D	501	-	-	7/7/7/7	-
2	HCS	С	501	-	-	3/7/7/7	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	501	HCS	CB-CG-SD	-4.81	108.73	113.74
2	С	501	HCS	CB-CG-SD	-4.63	108.92	113.74
2	В	501	HCS	CB-CG-SD	-4.40	109.16	113.74
2	А	501	HCS	CG-CB-CA	3.78	119.31	113.14
2	D	501	HCS	CB-CG-SD	-2.57	111.06	113.74

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	501	HCS	N-CA-CB-CG
2	А	501	HCS	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	В	501	HCS	CA-CB-CG-SD
2	С	501	HCS	N-CA-CB-CG
2	D	501	HCS	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	501	HCS	3	0
2	А	501	HCS	5	0
2	D	501	HCS	8	0
2	С	501	HCS	5	0

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		$OWAB(Å^2)$	Q<0.9	
1	А	391/398~(98%)	-0.26	22 (5%)	24	19	10, 23, 68, 96	0
1	В	395/398~(99%)	-0.26	27 (6%)	17	13	7, 21, 76, 88	0
1	С	391/398~(98%)	-0.33	20 (5%)	28	22	8, 22, 67, 91	0
1	D	391/398~(98%)	-0.12	22 (5%)	24	19	12, 30, 77, 92	0
All	All	1568/1592~(98%)	-0.25	91 (5%)	23	18	7, 24, 71, 96	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	59	TYR	10.9
1	А	51	ALA	8.7
1	А	52	GLY	8.5
1	С	55	ALA	8.4
1	D	53	GLU	8.1

6.2 Non-standard residues in protein, DNA, RNA chains (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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
1	LLP	А	211	24/25	0.97	0.15	11,17,20,21	0
1	LLP	В	211	24/25	0.98	0.11	9,14,16,17	0
1	LLP	С	211	24/25	0.98	0.15	10,19,23,26	0
1	LLP	D	211	24/25	0.98	0.13	17,21,24,26	0



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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	HCS	С	501	8/8	0.64	0.47	$90,\!90,\!91,\!92$	0
2	HCS	D	501	8/8	0.72	0.37	75,75,75,77	0
2	HCS	А	501	8/8	0.75	0.42	69,69,70,74	0
2	HCS	В	501	8/8	0.77	0.35	86,87,87,87	0

6.5 Other polymers (i)

There are no such residues in this entry.

