Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2024 – 07:14 AM EST

PDB ID	:	3LC0
Title	:	Histidyl-tRNA synthetase from Trypanosoma cruzi (Histidine complex)
Authors	:	Merritt, E.A.; Larson, E.T.; Medical Structural Genomics of Pathogenic Protozoa (MSGPP)
Deposited on	:	2010-01-08
Resolution	:	1.80 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 (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:

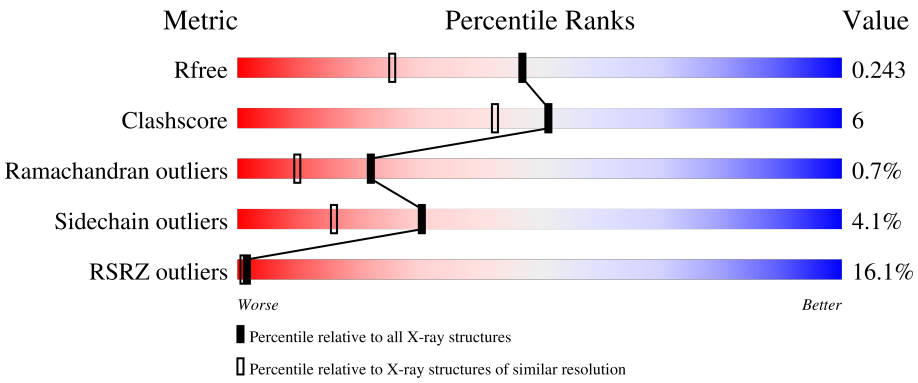
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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-RAY DIFFRACTION

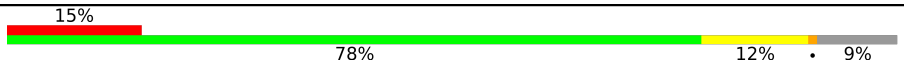
The reported resolution of this entry is 1.80 Å.

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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	A	456	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3485 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.

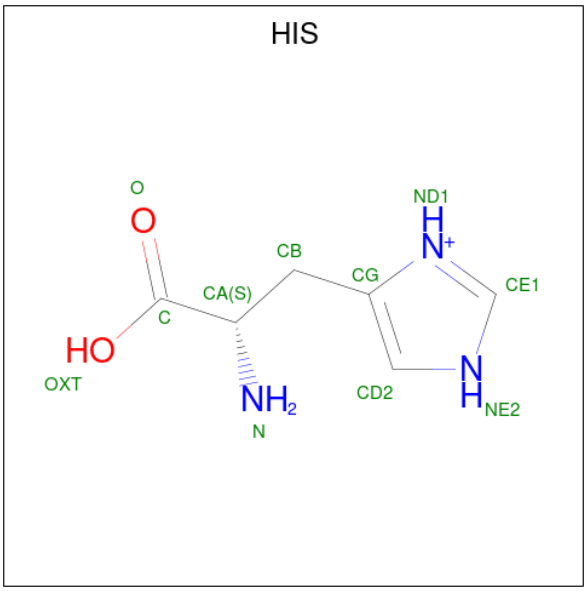
- Molecule 1 is a protein called Histidyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	415	3296	2111	561	604	20	0	8	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q4DA54
A	-20	ALA	-	expression tag	UNP Q4DA54
A	-19	HIS	-	expression tag	UNP Q4DA54
A	-18	HIS	-	expression tag	UNP Q4DA54
A	-17	HIS	-	expression tag	UNP Q4DA54
A	-16	HIS	-	expression tag	UNP Q4DA54
A	-15	HIS	-	expression tag	UNP Q4DA54
A	-14	HIS	-	expression tag	UNP Q4DA54
A	-13	MET	-	expression tag	UNP Q4DA54
A	-12	GLY	-	expression tag	UNP Q4DA54
A	-11	THR	-	expression tag	UNP Q4DA54
A	-10	LEU	-	expression tag	UNP Q4DA54
A	-9	GLU	-	expression tag	UNP Q4DA54
A	-8	ALA	-	expression tag	UNP Q4DA54
A	-7	GLN	-	expression tag	UNP Q4DA54
A	-6	THR	-	expression tag	UNP Q4DA54
A	-5	GLN	-	expression tag	UNP Q4DA54
A	-4	GLY	-	expression tag	UNP Q4DA54
A	-3	PRO	-	expression tag	UNP Q4DA54
A	-2	GLY	-	expression tag	UNP Q4DA54
A	-1	SER	-	expression tag	UNP Q4DA54
A	0	MET	-	expression tag	UNP Q4DA54

- Molecule 2 is HISTIDINE (three-letter code: HIS) (formula: $C_6H_{10}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	11	6	3	2	0	0

- Molecule 3 is water.

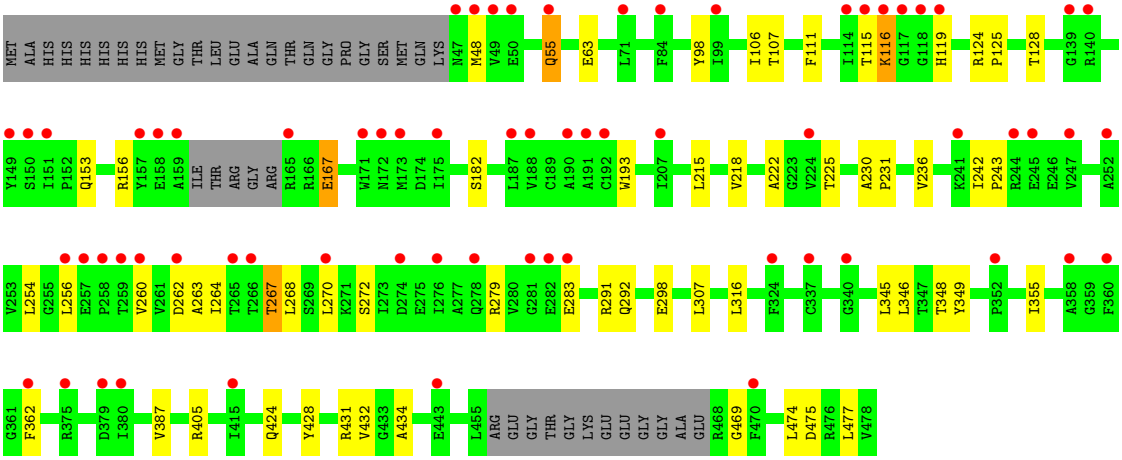
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	178	178	178	0	0

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: Histidyl-tRNA synthetase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	90.03Å 118.84Å 65.98Å 90.00° 132.57° 90.00°	Depositor
Resolution (Å)	34.11 – 1.80 33.94 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.11-1.80) 99.8 (33.94-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 1.81Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0096	Depositor
R, R_{free}	0.193 , 0.211 0.231 , 0.243	Depositor DCC
R_{free} test set	2374 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	32.6	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3485	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.56	0/3383	0.63	1/4584 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	124	ARG	NE-CZ-NH2	-5.10	117.75	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	3296	0	3282	37	1
2	A	11	0	6	2	0
3	A	178	0	0	8	1
All	All	3485	0	3288	37	1

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 6.

All (37) 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:193[A]:TRP:CE3	3:A:611:HOH:O	1.87	1.21
1:A:193[A]:TRP:HE3	3:A:611:HOH:O	1.34	0.89
1:A:424:GLN:HG3	3:A:654:HOH:O	1.74	0.88
1:A:263:ALA:O	1:A:267:THR:HG23	1.83	0.77
1:A:270:LEU:HD12	3:A:659:HOH:O	1.84	0.77
1:A:218:VAL:HG21	1:A:267:THR:HG21	1.76	0.67
1:A:119:HIS:HB3	3:A:641:HOH:O	2.01	0.60
1:A:405:ARG:NH2	1:A:475:ASP:OD1	2.35	0.60
1:A:236:VAL:HG13	1:A:268:LEU:HD11	1.84	0.59
1:A:292:GLN:NE2	3:A:639:HOH:O	2.35	0.59
1:A:128:THR:HG1	2:A:501:HIS:N	2.01	0.58
1:A:346[B]:LEU:HD23	1:A:355:ILE:HD12	1.84	0.58
1:A:230:ALA:HB3	1:A:231:PRO:HD3	1.88	0.56
1:A:231:PRO:HB2	1:A:254:LEU:HD21	1.89	0.55
1:A:267:THR:HG22	1:A:279:ARG:HH21	1.74	0.53
1:A:222:ALA:HB1	1:A:260:VAL:HG22	1.91	0.52
1:A:115:THR:O	1:A:116:LYS:HG3	2.10	0.51
1:A:63[A]:GLU:CD	1:A:63[A]:GLU:H	2.13	0.51
1:A:428:TYR:CZ	1:A:432:VAL:HG11	2.48	0.49
1:A:215:LEU:HD11	1:A:264:ILE:HG23	1.95	0.49
1:A:267:THR:HG22	1:A:279:ARG:NH2	2.28	0.48
1:A:345:LEU:O	1:A:348:THR:HB	2.14	0.46
1:A:193[A]:TRP:CZ3	3:A:611:HOH:O	2.41	0.46
1:A:242:ILE:HB	1:A:243:PRO:HD2	2.00	0.44
1:A:254:LEU:HD12	1:A:254:LEU:HA	1.87	0.43
1:A:431:ARG:NH1	3:A:640:HOH:O	2.51	0.43
1:A:316:LEU:CD1	2:A:501:HIS:HA	2.49	0.43
1:A:115:THR:OG1	1:A:116:LYS:N	2.52	0.42
1:A:236:VAL:CG1	1:A:268:LEU:HD11	2.47	0.42
1:A:387:VAL:HG23	1:A:434:ALA:HB2	2.01	0.42
1:A:98:TYR:CE1	1:A:125:PRO:HD2	2.56	0.41
1:A:106:ILE:HG23	1:A:107:THR:HG23	2.02	0.41
1:A:348:THR:HG22	1:A:349:TYR:HD1	1.85	0.41
1:A:477:LEU:HD12	1:A:477:LEU:HA	1.92	0.41
1:A:254:LEU:HB3	1:A:256:LEU:HD13	2.02	0.41
1:A:153:GLN:OE1	1:A:167:GLU:HG2	2.20	0.41
1:A:474:LEU:O	1:A:477:LEU:HB2	2.21	0.41

All (1) 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)
1:A:182:SER:CB	3:A:571:HOH:O[2_555]	1.94	0.26

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	417/456 (91%)	405 (97%)	9 (2%)	3 (1%)	22 10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	LYS
1	A	55	GLN
1	A	469	GLY

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	350/380 (92%)	335 (96%)	15 (4%)	29 14

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	MET
1	A	55	GLN
1	A	111	PHE

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Mol	Chain	Res	Type
1	A	156	ARG
1	A	167	GLU
1	A	225	THR
1	A	262	ASP
1	A	267	THR
1	A	272	SER
1	A	283	GLU
1	A	291	ARG
1	A	298[A]	GLU
1	A	298[B]	GLU
1	A	307	LEU
1	A	362	PHE

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

Mol	Chain	Res	Type
1	A	292	GLN
1	A	398	HIS

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)

1 ligand is 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HIS	A	501	-	6,11,11	0.93	1 (16%)	7,14,14	1.24	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
2	HIS	A	501	-	-	0/8/8/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HIS	OXT-C	-2.00	1.24	1.30

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HIS	2	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, 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	415/456 (91%)	0.84	67 (16%) 1 1	3, 13, 31, 44	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	ALA	7.5
1	A	48	MET	5.3
1	A	49	VAL	5.2
1	A	260	VAL	5.2
1	A	118	GLY	5.0
1	A	257	GLU	4.6
1	A	245	GLU	4.5
1	A	282	GLU	4.5
1	A	157	TYR	4.4
1	A	99	ILE	4.3
1	A	283	GLU	4.3
1	A	47	ASN	4.0
1	A	119	HIS	4.0
1	A	256	LEU	4.0
1	A	117	GLY	3.9
1	A	252	ALA	3.9
1	A	55	GLN	3.9
1	A	259	THR	3.9
1	A	151	ILE	3.8
1	A	171	TRP	3.8
1	A	360	PHE	3.7
1	A	270	LEU	3.7
1	A	115	THR	3.5
1	A	187	LEU	3.4
1	A	258	PRO	3.4
1	A	190	ALA	3.2
1	A	224	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	278	GLN	3.1
1	A	470	PHE	2.9
1	A	173	MET	2.9
1	A	207	ILE	2.9
1	A	362	PHE	2.9
1	A	139	GLY	2.9
1	A	84	PHE	2.9
1	A	158	GLU	2.7
1	A	352	PRO	2.7
1	A	191	ALA	2.6
1	A	114	ILE	2.6
1	A	262	ASP	2.5
1	A	175	ILE	2.5
1	A	324	PHE	2.5
1	A	116	LYS	2.4
1	A	281	GLY	2.4
1	A	358	ALA	2.4
1	A	140	ARG	2.4
1	A	337	CYS	2.4
1	A	274	ASP	2.4
1	A	165	ARG	2.4
1	A	375	ARG	2.3
1	A	188	VAL	2.3
1	A	265	THR	2.3
1	A	192	CYS	2.2
1	A	149	TYR	2.2
1	A	276	ILE	2.2
1	A	150[A]	SER	2.2
1	A	380	ILE	2.2
1	A	50	GLU	2.2
1	A	379	ASP	2.2
1	A	340	GLY	2.1
1	A	244	ARG	2.1
1	A	266	THR	2.1
1	A	415	ILE	2.1
1	A	247	VAL	2.1
1	A	241	LYS	2.1
1	A	172	ASN	2.1
1	A	443	GLU	2.1
1	A	71[A]	LEU	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 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	HIS	A	501	11/11	0.94	0.38	23,25,26,27	0

6.5 Other polymers (i)

There are no such residues in this entry.