Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 10:29 AM EST

PDB ID	:	4JJ7
Title	:	Caspase-3 specific unnatural amino acid-based peptides
Authors	:	Vickers, C.J.; Gonzalez-Paez, G.E.; Wolan, D.W.
Deposited on	:	2013-03-07
Resolution	:	1.18 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:

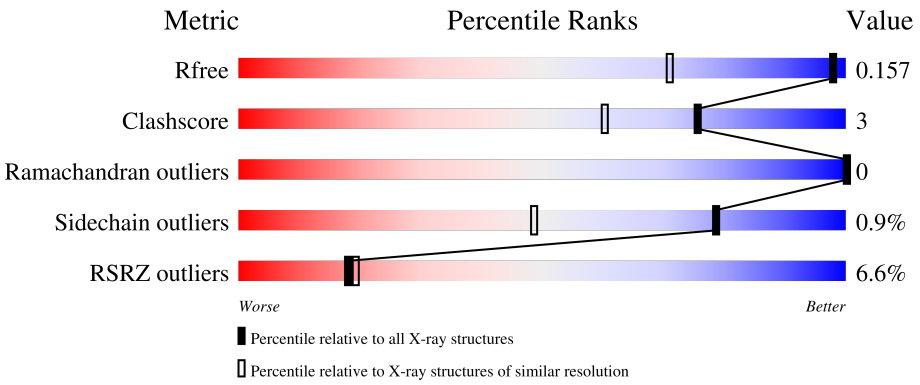
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.18 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	1123 (1.20-1.16)
Clashscore	141614	1182 (1.20-1.16)
Ramachandran outliers	138981	1134 (1.20-1.16)
Sidechain outliers	138945	1134 (1.20-1.16)
RSRZ outliers	127900	1102 (1.20-1.16)

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	275	6% 79% 7% • 12%
2	B	6	67% 17% 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2255 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 Caspase-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	241	1921	1214	326	365	16	0	6	0

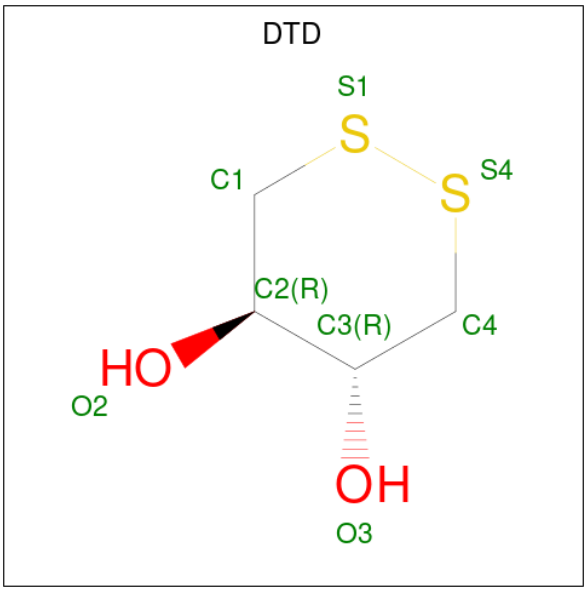
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	216	MET	-	initiating methionine	UNP Q14790
A	480	ALA	-	expression tag	UNP Q14790
A	481	ALA	-	expression tag	UNP Q14790
A	482	ALA	-	expression tag	UNP Q14790
A	483	LEU	-	expression tag	UNP Q14790
A	484	GLU	-	expression tag	UNP Q14790
A	485	HIS	-	expression tag	UNP Q14790
A	486	HIS	-	expression tag	UNP Q14790
A	487	HIS	-	expression tag	UNP Q14790
A	488	HIS	-	expression tag	UNP Q14790
A	489	HIS	-	expression tag	UNP Q14790
A	490	HIS	-	expression tag	UNP Q14790

- Molecule 2 is a protein called Caspase inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	49	33	6	10	0	0	0

- Molecule 3 is DITHIANE DIOL (three-letter code: DTD) (formula: $C_4H_8O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
3	A	1	8	4	2	2	0	0
			Total	C	O	S		
3	A	1	8	4	2	2	0	0

- Molecule 4 is water.

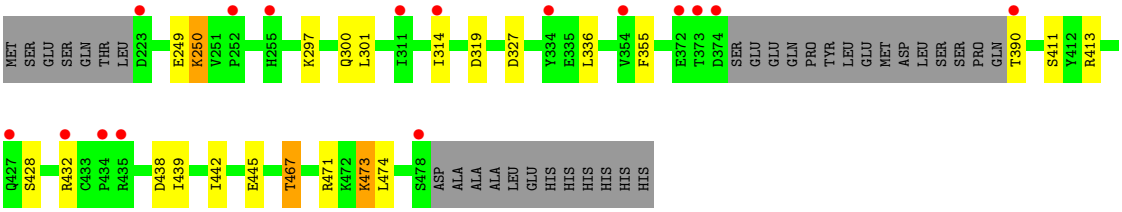
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	252	252	252	0	0
			Total	O		
4	B	17	17	17	0	0

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: Caspase-8

Chain A:



- Molecule 2: Caspase inhibitor

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	62.84Å 62.84Å 129.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.36 – 1.18 23.37 – 1.18	Depositor EDS
% Data completeness (in resolution range)	95.6 (23.36-1.18) 95.6 (23.37-1.18)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.64 (at 1.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.135 , 0.157 0.135 , 0.157	Depositor DCC
R_{free} test set	4672 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	12.0	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2255	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: HLX, DTD, 1U8, 1MH, ACE, B3L

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	0.74	2/1992 (0.1%)	0.89	8/2694 (0.3%)
2	B	0.53	0/7	2.07	0/8
All	All	0.74	2/1999 (0.1%)	0.89	8/2702 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	411	SER	CB-OG	-8.54	1.31	1.42
1	A	355	PHE	CD2-CE2	5.42	1.50	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	471	ARG	NE-CZ-NH2	9.09	124.84	120.30
1	A	471	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	A	327	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	319	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	467[A]	THR	CA-CB-CG2	-6.14	103.81	112.40
1	A	467[B]	THR	CA-CB-CG2	-6.14	103.81	112.40
1	A	473	LYS	CD-CE-NZ	5.42	124.17	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	327	ASP	CB-CG-OD1	-5.05	113.76	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	413	ARG	Sidechain
2	B	504	B3L	Mainchain,Peptide

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	1921	0	1879	11	0
2	B	49	0	38	1	0
3	A	16	0	16	0	0
4	A	252	0	0	2	0
4	B	17	0	0	1	0
All	All	2255	0	1933	12	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 3.

All (12) 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:467[B]:THR:HG23	4:A:845:HOH:O	1.89	0.73
1:A:473:LYS:NZ	4:A:996:HOH:O	2.04	0.72
1:A:314[A]:ILE:CD1	1:A:336:LEU:HD13	2.32	0.59
1:A:439:ILE:HG21	1:A:474:LEU:HD23	1.89	0.55
1:A:432:ARG:NH2	1:A:445:GLU:OE1	2.38	0.55
1:A:432:ARG:HE	1:A:445:GLU:CD	2.12	0.52
1:A:428[A]:SER:OG	1:A:442:ILE:HG23	2.11	0.49
2:B:504:B3L:H2E1	4:B:611:HOH:O	2.14	0.47
1:A:297:LYS:HD3	1:A:300:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLU:HG3	1:A:250:LYS:HE3	2.03	0.41
1:A:438:ASP:HB3	1:A:473:LYS:HE2	2.03	0.41
1:A:297:LYS:HD2	1:A:301:LEU:HD11	2.04	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	243/275 (88%)	236 (97%)	7 (3%)	0	100	100
2	B	1/6 (17%)	1 (100%)	0	0	100	100
All	All	244/281 (87%)	237 (97%)	7 (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	218/247 (88%)	216 (99%)	2 (1%)	78	49
2	B	1/1 (100%)	1 (100%)	0	100	100
All	All	219/248 (88%)	217 (99%)	2 (1%)	78	49

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	LYS
1	A	390	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HLX	B	505	2	7,8,9	2.01	2 (28%)	4,9,11	1.80	2 (50%)
2	B3L	B	504	2	8,8,9	1.32	1 (12%)	7,9,11	1.67	2 (28%)
2	1U8	B	506	2,1	6,8,20	0.88	0	5,10,27	1.02	0
2	1MH	B	502	2	10,11,12	0.63	0	10,13,15	0.84	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	HLX	B	505	2	-	0/6/7/9	-
2	B3L	B	504	2	-	0/7/7/8	-
2	1U8	B	506	2,1	-	0/7/8/17	-
2	1MH	B	502	2	-	0/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	505	HLX	CB-CA	-4.69	1.47	1.53
2	B	504	B3L	CG-CA	-2.92	1.48	1.53
2	B	505	HLX	CG-CB	-2.37	1.46	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	505	HLX	C9-C7-C8	-2.60	98.54	110.51
2	B	505	HLX	CB-CG-C7	-2.44	108.22	114.61
2	B	504	B3L	O-C-CB	-2.31	118.69	125.43
2	B	504	B3L	CG-CA-CB	2.05	116.83	111.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	504	B3L	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DTD	A	601	-	6,8,8	1.81	2 (33%)	6,10,10	1.59	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DTD	A	602	-	6,8,8	1.18	1 (16%)	6,10,10	1.08	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	DTD	A	601	-	-	-	0/0/1/1
3	DTD	A	602	-	-	-	0/0/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	DTD	C3-C2	3.12	1.56	1.52
3	A	601	DTD	O3-C3	-2.14	1.38	1.43
3	A	602	DTD	O3-C3	-2.01	1.39	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	DTD	O3-C3-C4	-2.17	106.17	109.91

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 (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	241/275 (87%)	0.70	16 (6%) 18 19	9, 13, 24, 35	0
2	B	1/6 (16%)	0.96	0 100 100	15, 15, 15, 15	0
All	All	242/281 (86%)	0.70	16 (6%) 18 19	9, 13, 24, 35	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	373	THR	7.8
1	A	390	THR	6.3
1	A	478	SER	5.4
1	A	374	ASP	4.2
1	A	435	ARG	4.0
1	A	434	PRO	3.0
1	A	372	GLU	2.9
1	A	427	GLN	2.8
1	A	432	ARG	2.5
1	A	223	ASP	2.4
1	A	311	ILE	2.3
1	A	354	VAL	2.3
1	A	252	PRO	2.2
1	A	314[A]	ILE	2.2
1	A	255	HIS	2.1
1	A	334	TYR	2.0

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, 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	B3L	B	504	9/10	0.96	0.10	11,14,21,22	0
2	1MH	B	502	11/12	0.97	0.07	11,12,13,13	0
2	HLX	B	505	9/10	0.97	0.10	11,13,23,27	0
2	1U8	B	506	9/20	0.98	0.09	10,10,11,15	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, 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
3	DTD	A	601	8/8	0.96	0.18	21,25,27,30	0
3	DTD	A	602	8/8	0.98	0.08	14,15,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.