



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:01 AM UTC

PDB ID : 1J1D / pdb_00001j1d
Title : Crystal structure of the 46kDa domain of human cardiac troponin in the Ca²⁺ saturated form
Authors : Takeda, S.; Yamashita, A.; Maeda, K.; Maeda, Y.
Deposited on : 2002-12-03
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

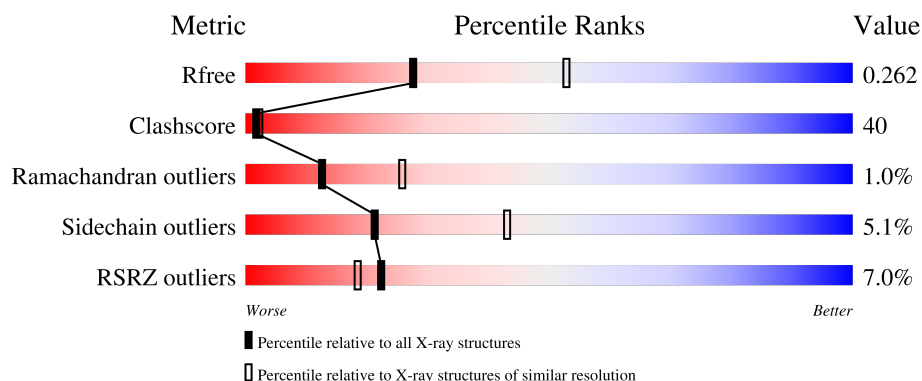
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (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 $\leq 5\%$. 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	161	8% 45% 47% 7%
1	D	161	11% 46% 46% 7%
2	B	106	2% 35% 28% 34%
2	E	106	2% 37% 29% 29%
3	C	133	6% 48% 34% 7% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	133	5% 40% 40% 7% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5777 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 Troponin C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1269	786	193	279	11			
1	D	160	Total	C	N	O	S	0	0	0
			1274	789	195	280	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	SER	CYS	engineered mutation	UNP P63316
A	84	SER	CYS	engineered mutation	UNP P63316
D	35	SER	CYS	engineered mutation	UNP P63316
D	84	SER	CYS	engineered mutation	UNP P63316

- Molecule 2 is a protein called Troponin T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	70	Total	C	N	O		0	0	0
			611	383	114	114				
2	E	75	Total	C	N	O		0	0	0
			656	411	125	120				

- Molecule 3 is a protein called Troponin I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	118	Total	C	N	O	S	0	0	0
			942	584	180	176	2			
3	F	116	Total	C	N	O	S	0	0	0
			917	569	172	174	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	31	MET	THR	engineered mutation	UNP P19429
C	80	ALA	CYS	engineered mutation	UNP P19429
C	97	ALA	CYS	engineered mutation	UNP P19429
F	31	MET	THR	engineered mutation	UNP P19429
F	80	ALA	CYS	engineered mutation	UNP P19429
F	97	ALA	CYS	engineered mutation	UNP P19429

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Ca 3 3	0	0
4	D	3	Total Ca 3 3	0	0

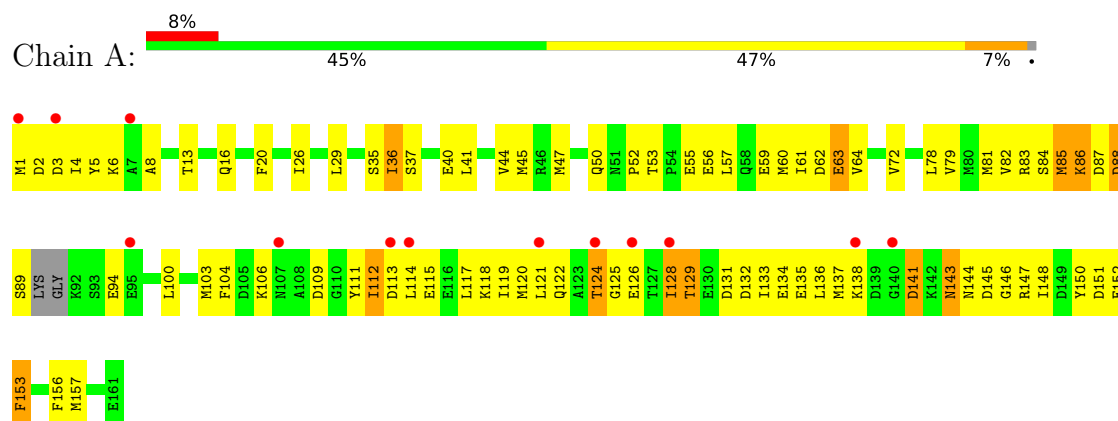
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	18	Total O 18 18	0	0
5	B	21	Total O 21 21	0	0
5	C	15	Total O 15 15	0	0
5	D	14	Total O 14 14	0	0
5	E	20	Total O 20 20	0	0
5	F	14	Total O 14 14	0	0

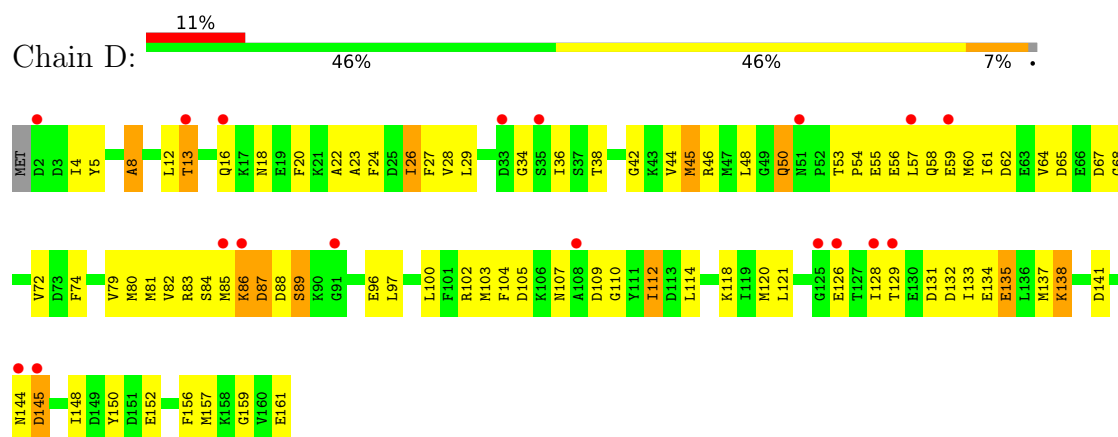
3 Residue-property plots

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.

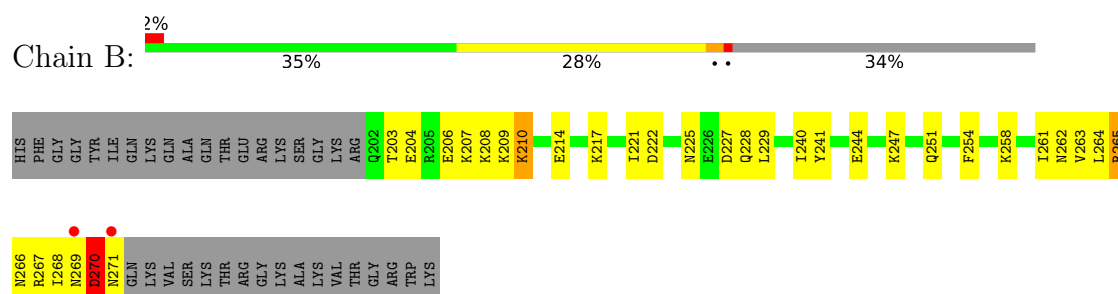
• Molecule 1: Troponin C



• Molecule 1: Troponin C



• Molecule 2: Troponin T



Chain E:

2% 37% 29% 29%

HIS PHE GLY GLY TYR ILE GLN LYS GLN ALA THR GLU ARG LYS SER GLY K200 R201 Q202 T203 E204 R205 E206 K209 K210 E214 K217 T221 D222 N225 Q228 L229 R230 Q238 T239 T240 Y241 N242 L243 E244 A245 E246 K247 F248 F254 R255 Q256 K257 Q258 Y259 E260

Chain C:

0.15
0.10
0.05
0.00

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200

MET GLU PRO HIS K36 K37 K38 S39 K40 T41 S42 S44 R45 K46 L47 Q48 L49 K50 T51 L52 L53 L54 Q55 L56 A57 E60 L61 E62 R63 E64 A65 G70 R74 A75 L76 S77 T78 A91 E92 L93 Q94 D95 Q99 A102 R103 K106 V107 E110 V100

Chain F:

Amino Acid	Percentage
MET	5%
GLU	
PRO	
HIS	
ALA	
LYS	
K37	
K38	
S39	
K40	
I41	
S44	
R45	
K46	
L47	
Q48	
L49	
K50	
T51	
L52	
L53	
L54	
Q55	
I56	
A57	
E60	
L61	
E62	
R63	
E64	
A65	
E66	
E67	
R68	
R69	
K72	
L76	
Q81	
P82	
L83	
E84	
L85	
A86	
G87	
L88	
G89	
F90	
A91	
E92	
L93	
Q94	
Q95	
R98	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.35Å 167.86Å 69.71Å 90.00° 101.35° 90.00°	Depositor
Resolution (Å)	40.00 – 2.61 40.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	96.3 (40.00-2.61) 96.3 (40.00-2.61)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.264 , 0.298 0.264 , 0.262	Depositor DCC
R_{free} test set	948 reflections (3.40%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5777	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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: CA

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	0/1281	1.07	9/1711 (0.5%)
1	D	0.46	0/1287	1.09	7/1720 (0.4%)
2	B	0.59	0/617	1.00	5/821 (0.6%)
2	E	0.56	0/662	1.06	6/879 (0.7%)
3	C	0.55	0/945	1.08	7/1257 (0.6%)
3	F	0.56	0/920	1.10	9/1224 (0.7%)
All	All	0.54	0/5712	1.07	43/7612 (0.6%)

There are no bond length outliers.

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	38	LYS	N-CA-C	10.06	124.14	110.55
1	D	87	ASP	N-CA-C	9.77	126.51	107.57
1	D	145	ASP	N-CA-C	-9.69	100.97	113.17
3	C	63	ARG	N-CA-C	-9.48	101.03	111.36
1	D	89	SER	N-CA-C	8.23	121.87	110.35

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	1269	0	1197	133	0
1	D	1274	0	1202	144	0
2	B	611	0	628	39	0
2	E	656	0	684	58	0
3	C	942	0	1002	91	0
3	F	917	0	970	121	0
4	A	3	0	0	0	0
4	D	3	0	0	0	0
5	A	18	0	0	3	0
5	B	21	0	0	1	0
5	C	15	0	0	2	0
5	D	14	0	0	1	0
5	E	20	0	0	1	0
5	F	14	0	0	0	0
All	All	5777	0	5683	458	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 40.

The worst 5 of 458 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:D:4:ILE:HD11	1:D:159:GLY:HA3	1.28	1.09
1:A:104:PHE:HA	1:A:120:MET:HE3	1.37	1.07
1:A:135:GLU:HG3	3:C:41:ILE:HG22	1.37	1.03
3:F:88:LEU:HD22	3:F:92:GLU:HB2	1.41	1.02
1:D:121:LEU:HB3	1:D:128:ILE:CD1	1.89	1.01

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	155/161 (96%)	141 (91%)	11 (7%)	3 (2%)	6	12
1	D	158/161 (98%)	135 (85%)	22 (14%)	1 (1%)	21	39
2	B	68/106 (64%)	62 (91%)	5 (7%)	1 (2%)	8	16
2	E	73/106 (69%)	68 (93%)	5 (7%)	0	100	100
3	C	114/133 (86%)	104 (91%)	10 (9%)	0	100	100
3	F	112/133 (84%)	101 (90%)	9 (8%)	2 (2%)	6	13
All	All	680/800 (85%)	611 (90%)	62 (9%)	7 (1%)	12	26

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	GLY
1	A	63	GLU
2	B	270	ASP
1	A	141	ASP
1	D	86	LYS

5.3.2 Protein sidechains ⓘ

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	141/142 (99%)	137 (97%)	4 (3%)	38	64
1	D	141/142 (99%)	135 (96%)	6 (4%)	26	49
2	B	66/95 (70%)	63 (96%)	3 (4%)	24	48
2	E	71/95 (75%)	67 (94%)	4 (6%)	19	39
3	C	98/110 (89%)	91 (93%)	7 (7%)	13	29
3	F	95/110 (86%)	88 (93%)	7 (7%)	13	27
All	All	612/694 (88%)	581 (95%)	31 (5%)	21	43

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	13	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	114	ILE
1	D	112	ILE
3	F	149	ILE
3	F	56	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	101	HIS
3	C	156	GLN
3	F	55	GLN
2	E	242	ASN
2	E	272	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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 [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	159/161 (98%)	0.79	13 (8%) 17 14	44, 73, 95, 114	0
1	D	160/161 (99%)	0.80	18 (11%) 10 8	51, 85, 106, 111	0
2	B	70/106 (66%)	0.25	2 (2%) 53 48	42, 55, 77, 85	0
2	E	75/106 (70%)	0.32	2 (2%) 56 51	38, 61, 103, 108	0
3	C	118/133 (88%)	0.69	8 (6%) 23 19	43, 72, 104, 110	0
3	F	116/133 (87%)	0.68	6 (5%) 33 27	41, 72, 101, 113	0
All	All	698/800 (87%)	0.65	49 (7%) 22 18	38, 73, 103, 114	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	271	ASN	4.2
3	F	161	ALA	3.9
1	D	86	LYS	3.5
1	A	124	THR	3.5
1	A	121	LEU	3.4

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 oligosaccharides 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
4	CA	A	201	1/1	0.95	0.13	68,68,68,68	0
4	CA	A	203	1/1	0.96	0.07	95,95,95,95	0
4	CA	D	203	1/1	0.96	0.07	79,79,79,79	0
4	CA	D	201	1/1	0.97	0.05	92,92,92,92	0
4	CA	D	202	1/1	0.98	0.04	79,79,79,79	0
4	CA	A	202	1/1	0.99	0.04	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.