



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:16 pm BST

PDB ID : 5MWC
Title : Crystal structure of the genetically-encoded green calcium indicator NTnC in its calcium bound state
Authors : Boyko, K.M.; Nikolaeva, A.Y.; Korzhenevskiy, D.A.; Rakitina, T.V.; Popov, V.O.; Subach, O.M.; Barykina, N.V.; Subach, F.V.
Deposited on : 2017-01-18
Resolution : 2.45 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

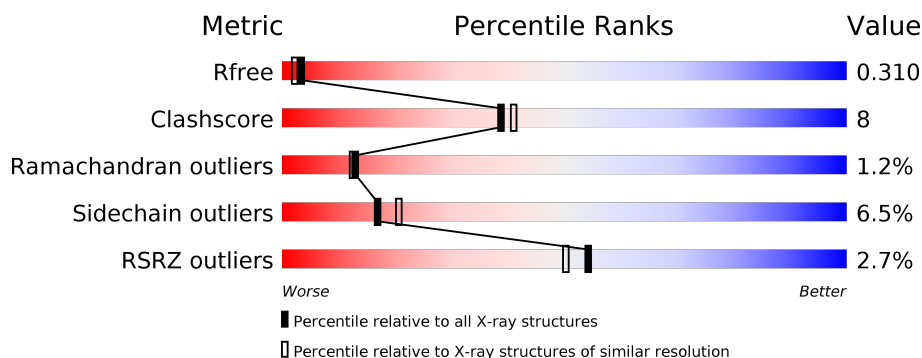
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 on 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	309	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>15%</div> <div>•</div> <div>18%</div> </div> </div>
1	D	309	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4161 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 genetically-encoded green calcium indicator NTnC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	276	Total	C	N	O	S	0	0	0
			2164	1373	358	420	13			
1	A	254	Total	C	N	O	S	0	0	0
			1948	1239	324	373	12			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	D	2	Total	Ca	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	26	Total	O	0	0
			26	26		
3	A	20	Total	O	0	0
			20	20		

- Molecule 1: genetically-encoded green calcium indicator NTnC



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.10 Å 82.10 Å 157.47 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.80 – 2.45 46.73 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (72.80-2.45) 99.7 (46.73-2.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.45 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.239 , 0.310 0.239 , 0.310	Depositor DCC
R_{free} test set	1063 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	59.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4161	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: CR2, 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	0.61	0/1978	0.87	2/2681 (0.1%)
1	D	0.58	0/2200	0.83	5/2979 (0.2%)
All	All	0.60	0/4178	0.85	7/5660 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	291	LEU	CA-CB-CG	7.50	132.54	115.30
1	D	291	LEU	CB-CG-CD1	-6.66	99.68	111.00
1	D	291	LEU	CB-CG-CD2	6.65	122.30	111.00
1	A	291	LEU	CA-CB-CG	6.44	130.12	115.30
1	A	210	LEU	CB-CA-C	5.88	121.37	110.20
1	D	98	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	D	197	ASP	CB-CG-OD2	-5.48	113.37	118.30

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	1948	0	1757	31	0
1	D	2164	0	1990	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	D	2	0	0	0	0
3	A	20	0	0	0	0
3	D	26	0	0	0	0
All	All	4161	0	3747	59	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 8.

All (59) 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:231:PRO:HD2	1:D:235:THR:HG23	1.57	0.86
1:D:174:GLY:O	1:D:177:ILE:HG12	1.78	0.84
1:D:205:ASP:N	1:D:208:GLU:OE1	2.13	0.76
1:A:156:CYS:O	1:A:157:PHE:HB2	1.87	0.74
1:D:176:ILE:HG22	1:D:177:ILE:N	2.06	0.70
1:A:206:PHE:O	1:A:208:GLU:N	2.21	0.70
1:A:206:PHE:C	1:A:208:GLU:H	1.94	0.70
1:A:97:HIS:HD2	1:A:111:ASN:HD21	1.41	0.68
1:A:151:GLU:O	1:A:154:SER:OG	2.14	0.65
1:D:102:PHE:CD1	1:D:254:SER:HB3	2.31	0.65
1:A:189:PRO:HA	1:A:192:ILE:HG23	1.78	0.64
1:D:170:ARG:NH1	1:D:190:ASP:OD1	2.32	0.62
1:A:102:PHE:CD1	1:A:254:SER:HB3	2.35	0.62
1:A:97:HIS:CD2	1:A:111:ASN:HD21	2.17	0.61
1:D:229:ALA:HA	1:D:274:GLN:HG3	1.84	0.60
1:A:32:MET:CE	1:A:291:LEU:HD13	2.32	0.60
1:A:149:SER:HB3	1:A:241:LYS:HG3	1.85	0.59
1:D:154:SER:HA	1:D:206:PHE:CE1	2.40	0.57
1:D:34:GLY:HA3	1:D:48:ASN:O	2.05	0.56
1:A:34:GLY:HA3	1:A:48:ASN:O	2.05	0.56
1:D:154:SER:HA	1:D:206:PHE:HE1	1.71	0.56
1:D:204:ILE:HA	1:D:208:GLU:OE1	2.08	0.54
1:A:206:PHE:C	1:A:208:GLU:N	2.62	0.53
1:D:73:GLN:O	1:D:85:GLN:HG3	2.07	0.53
1:A:73:GLN:O	1:A:85:GLN:HG3	2.09	0.53
1:A:233:ASP:HA	1:A:271:LEU:HD21	1.91	0.52
1:D:149:SER:OG	1:D:151:GLU:HG2	2.09	0.52
1:D:193:PHE:CZ	1:D:203:ARG:HA	2.44	0.52
1:D:169:ASP:H	1:D:172:GLU:CG	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ILE:O	1:A:28:VAL:HG12	2.11	0.51
1:D:176:ILE:HG22	1:D:177:ILE:H	1.73	0.51
1:D:234:LYS:NZ	1:D:265:PRO:HD3	2.26	0.50
1:D:284:LEU:HD11	1:D:291:LEU:HD23	1.94	0.50
1:D:176:ILE:CG2	1:D:177:ILE:N	2.75	0.50
1:D:32:MET:CE	1:D:291:LEU:HD12	2.43	0.49
1:A:189:PRO:HA	1:A:192:ILE:CG2	2.43	0.48
1:A:32:MET:HE1	1:A:291:LEU:HD13	1.95	0.47
1:A:70:CR2:HD1	1:A:70:CR2:N2	2.29	0.47
1:A:98:ARG:HB3	1:A:110:VAL:CG1	2.45	0.47
1:A:45:GLU:HG2	1:A:74:TYR:CD2	2.49	0.47
1:D:98:ARG:HD3	1:D:258:THR:OG1	2.15	0.47
1:D:193:PHE:HZ	1:D:203:ARG:HA	1.80	0.46
1:D:45:GLU:HG2	1:D:74:TYR:CD2	2.50	0.46
1:D:250:LYS:HE2	1:D:251:ARG:H	1.80	0.45
1:D:169:ASP:H	1:D:172:GLU:HG2	1.80	0.45
1:A:156:CYS:O	1:A:157:PHE:CB	2.63	0.44
1:D:73:GLN:O	1:D:85:GLN:CG	2.66	0.44
1:D:49:LEU:HD12	1:D:291:LEU:HD13	1.98	0.43
1:A:271:LEU:O	1:A:274:GLN:HG2	2.19	0.43
1:A:90:ASP:OD1	1:A:92:SER:OG	2.30	0.43
1:A:98:ARG:HD3	1:A:258:THR:OG1	2.18	0.43
1:A:73:GLN:O	1:A:85:GLN:CG	2.67	0.42
1:D:230:CYS:H	1:D:274:GLN:CD	2.23	0.42
1:A:192:ILE:HG13	1:A:193:PHE:N	2.35	0.41
1:A:102:PHE:HD1	1:A:254:SER:HB3	1.84	0.41
1:A:228:MET:HB3	1:A:236:LEU:HD21	2.03	0.41
1:A:98:ARG:HB3	1:A:110:VAL:HG13	2.02	0.40
1:A:62:ILE:HD12	1:A:62:ILE:HA	1.96	0.40
1:A:77:TYR:CZ	1:A:276:MET:HG2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	241/309 (78%)	228 (95%)	8 (3%)	5 (2%)	7	5
1	D	267/309 (86%)	259 (97%)	7 (3%)	1 (0%)	34	41
All	All	508/618 (82%)	487 (96%)	15 (3%)	6 (1%)	13	12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	PHE
1	A	169	ILE
1	A	207	ASP
1	D	177	ILE
1	A	209	PHE
1	A	303	VAL

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	193/265 (73%)	182 (94%)	11 (6%)	20	26
1	D	224/265 (84%)	208 (93%)	16 (7%)	14	17
All	All	417/530 (79%)	390 (94%)	27 (6%)	17	21

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	115	THR
1	D	124	GLU
1	D	150	GLU
1	D	154	SER
1	D	158	ARG
1	D	162	LYS
1	D	169	ASP

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Mol	Chain	Res	Type
1	D	170	ARG
1	D	178	ARG
1	D	207	ASP
1	D	220	MET
1	D	250	LYS
1	D	254	SER
1	D	271	LEU
1	D	274	GLN
1	D	301	THR
1	A	101	GLN
1	A	107	SER
1	A	124	GLU
1	A	157	PHE
1	A	169	ILE
1	A	170	ASP
1	A	192	ILE
1	A	207	ASP
1	A	255	THR
1	A	264	LYS
1	A	301	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	35	GLN
1	D	72	HIS
1	A	35	GLN
1	A	72	HIS
1	A	97	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 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
1	CR2	A	70	1	20,20,21	3.74	5 (25%)	25,27,29	5.27	10 (40%)
1	CR2	D	70	1	20,20,21	3.23	4 (20%)	25,27,29	4.48	10 (40%)

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
1	CR2	A	70	1	-	0/6/25/26	0/2/2/2
1	CR2	D	70	1	-	0/6/25/26	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	CR2	CB2-CA2	15.08	1.47	1.35
1	D	70	CR2	CB2-CA2	13.06	1.46	1.35
1	A	70	CR2	C1-N2	3.51	1.38	1.32
1	D	70	CR2	CA2-C2	-3.32	1.45	1.48
1	A	70	CR2	C2-N3	-3.10	1.32	1.39
1	D	70	CR2	C2-N3	-2.86	1.33	1.39
1	A	70	CR2	CA2-C2	-2.52	1.46	1.48
1	D	70	CR2	C1-N2	2.33	1.36	1.32
1	A	70	CR2	CA2-N2	-2.28	1.33	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	CR2	CA2-C2-N3	17.66	111.72	103.37
1	D	70	CR2	CA2-C2-N3	13.63	109.82	103.37
1	A	70	CR2	O2-C2-CA2	-13.52	123.37	130.96
1	D	70	CR2	O2-C2-CA2	-13.06	123.62	130.96
1	A	70	CR2	C2-N3-C1	-7.89	104.14	107.99
1	D	70	CR2	C2-N3-C1	-7.48	104.33	107.99
1	A	70	CR2	CB2-CA2-C2	6.90	130.52	122.28
1	A	70	CR2	C2-CA2-N2	-6.32	104.51	108.93
1	D	70	CR2	C1-CA1-N1	-4.33	103.28	112.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	CR2	O3-C3-CA3	-3.76	115.03	126.39
1	D	70	CR2	O3-C3-CA3	-3.75	115.07	126.39
1	D	70	CR2	CB2-CA2-C2	3.71	126.70	122.28
1	D	70	CR2	C2-CA2-N2	-2.80	106.97	108.93
1	A	70	CR2	CB2-CA2-N2	-2.78	124.97	128.83
1	A	70	CR2	C1-CA1-N1	-2.56	107.19	112.85
1	D	70	CR2	CD2-CG2-CD1	2.54	121.39	117.64
1	A	70	CR2	CG2-CB2-CA2	-2.48	126.91	129.94
1	D	70	CR2	CE2-CD2-CG2	-2.26	118.30	121.25
1	D	70	CR2	CD2-CG2-CB2	-2.11	114.03	121.22
1	A	70	CR2	CA1-C1-N3	2.03	125.23	122.52

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
1	A	70	CR2	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	253/309 (81%)	0.10	6 (2%) 59 54	37, 61, 99, 116	0
1	D	275/309 (88%)	0.07	8 (2%) 51 47	35, 64, 91, 104	0
All	All	528/618 (85%)	0.08	14 (2%) 54 50	35, 62, 95, 116	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	169	ASP	4.8
1	A	170	ASP	4.8
1	D	193	PHE	3.3
1	D	176	ILE	2.9
1	A	127	VAL	2.6
1	A	157	PHE	2.6
1	D	255	THR	2.4
1	D	174	GLY	2.2
1	D	160	PHE	2.2
1	D	52	THR	2.2
1	A	263	ALA	2.1
1	A	54	GLY	2.1
1	A	159	THR	2.0
1	D	25	ILE	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(\AA^2)	Q<0.9
1	CR2	A	70	19/20	0.96	0.13	33,39,56,60	0
1	CR2	D	70	19/20	0.98	0.12	34,36,40,40	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
2	CA	A	401	1/1	0.88	0.16	88,88,88,88	0
2	CA	D	401	1/1	0.97	0.11	84,84,84,84	0
2	CA	D	402	1/1	0.97	0.07	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.