



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 12:28 AM EDT

PDB ID : 2H2U
Title : Crystal structure of the E130Y mutant of human soluble calcium-activated nucleotidase (SCAN) with calcium ion
Authors : Yang, M.; Horii, K.; Herr, A.B.; Kirley, T.L.
Deposited on : 2006-05-19
Resolution : 2.40 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 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

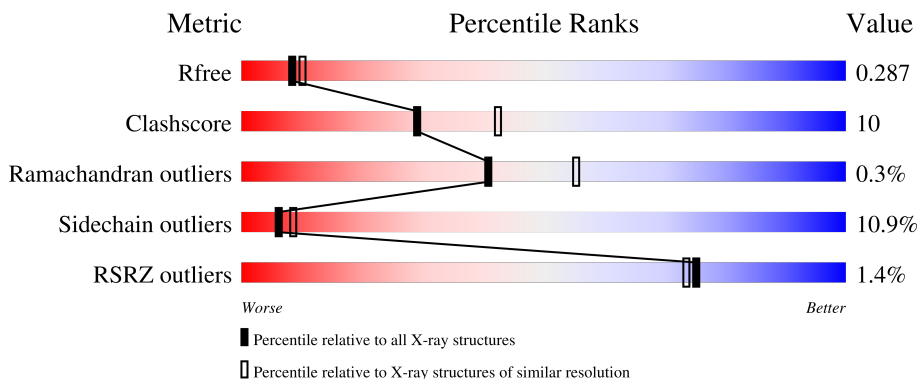
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	339	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">72% 19% • 7%</p>
1	B	339	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">67% 23% • 6%</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5035 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 Soluble calcium-activated nucleotidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	315	2491	1588	417	483	3	0	0	0
1	B	317	2513	1603	421	486	3	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	cloning artifact	UNP Q8WVQ1
A	-6	SER	-	cloning artifact	UNP Q8WVQ1
A	-5	HIS	-	cloning artifact	UNP Q8WVQ1
A	-4	MET	-	cloning artifact	UNP Q8WVQ1
A	-3	ALA	-	cloning artifact	UNP Q8WVQ1
A	-2	SER	-	cloning artifact	UNP Q8WVQ1
A	90	TYR	GLU	engineered mutation	UNP Q8WVQ1
B	-7	GLY	-	cloning artifact	UNP Q8WVQ1
B	-6	SER	-	cloning artifact	UNP Q8WVQ1
B	-5	HIS	-	cloning artifact	UNP Q8WVQ1
B	-4	MET	-	cloning artifact	UNP Q8WVQ1
B	-3	ALA	-	cloning artifact	UNP Q8WVQ1
B	-2	SER	-	cloning artifact	UNP Q8WVQ1
B	90	TYR	GLU	engineered mutation	UNP Q8WVQ1

- 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	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total 18	O 18	0	0
3	B	11	Total 11	O 11	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.89Å 52.41Å 77.81Å 100.94° 106.51° 99.32°	Depositor
Resolution (Å)	47.04 – 2.40 47.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.5 (47.04-2.40) 86.5 (47.01-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.216 , 0.285 0.217 , 0.287	Depositor DCC
R_{free} test set	1075 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtrriage
Anisotropy	0.080	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5035	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% 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	0.61	0/2554	0.72	0/3468
1	B	0.56	0/2578	0.71	1/3502 (0.0%)
All	All	0.59	0/5132	0.71	1/6970 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	ASP	CB-CG-OD1	5.15	122.93	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	2491	0	2405	40	0
1	B	2513	0	2421	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	18	0	0	0	0
3	B	11	0	0	0	0
All	All	5035	0	4826	94	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 10.

All (94) 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:93:ARG:HH21	1:B:93:ARG:HG2	1.10	1.11
1:A:230:ARG:HH11	1:A:230:ARG:HG3	0.95	1.10
1:B:230:ARG:HG3	1:B:230:ARG:HH11	1.17	1.10
1:B:28:ARG:HD2	1:B:33:ILE:HD13	1.46	0.96
1:A:230:ARG:HG3	1:A:230:ARG:NH1	1.76	0.95
1:B:34:ARG:HG2	1:B:65:THR:HG22	1.48	0.94
1:A:230:ARG:HH11	1:A:230:ARG:CG	1.79	0.94
1:B:34:ARG:CG	1:B:65:THR:HG22	2.00	0.91
1:B:230:ARG:HH11	1:B:230:ARG:CG	1.86	0.88
1:A:240:LYS:H	1:A:240:LYS:HE2	1.40	0.87
1:B:93:ARG:HG2	1:B:93:ARG:NH2	1.90	0.76
1:B:36:ARG:HG3	1:B:331:ILE:HG13	1.68	0.75
1:B:93:ARG:HH21	1:B:93:ARG:CG	1.99	0.70
1:A:138:VAL:HG12	1:A:140:LYS:H	1.57	0.69
1:A:111:ASP:OD2	1:A:114:THR:OG1	2.05	0.68
1:A:42:ASP:HB2	1:A:326:GLU:HG3	1.76	0.68
1:B:230:ARG:HG3	1:B:230:ARG:NH1	1.93	0.67
1:B:23:LEU:HB2	1:B:331:ILE:HG22	1.77	0.67
1:B:34:ARG:HG3	1:B:65:THR:HG22	1.79	0.65
1:B:58:TYR:HB2	1:B:82:GLY:O	1.96	0.64
1:A:139:GLU:OE1	1:B:124:LYS:HB3	1.97	0.64
1:A:71:ASP:HA	1:A:312:ARG:HH22	1.63	0.63
1:A:93:ARG:HB3	1:A:113:ARG:HG3	1.78	0.63
1:B:200:ARG:HD2	1:B:205:ILE:O	1.99	0.63
1:A:248:ASN:HB2	1:A:265:VAL:O	1.99	0.62
1:A:179:LYS:NZ	1:A:189:HIS:ND1	2.48	0.60
1:B:24:SER:N	1:B:331:ILE:OXT	2.34	0.60
1:A:42:ASP:CB	1:A:326:GLU:HG3	2.31	0.59
1:B:220:ASP:O	1:B:223:GLN:OE1	2.22	0.57
1:B:131:LEU:HD22	1:B:179:LYS:HG2	1.87	0.57
1:A:283:THR:O	1:A:284:ASP:HB2	2.06	0.56
1:B:138:VAL:HG12	1:B:140:LYS:H	1.71	0.56
1:B:240:LYS:H	1:B:240:LYS:HE2	1.70	0.56
1:B:300:VAL:HG21	1:B:324:LYS:HD3	1.89	0.54
1:B:93:ARG:NH2	1:B:93:ARG:CG	2.66	0.54
1:A:240:LYS:HE2	1:A:240:LYS:N	2.18	0.54
1:A:79:LYS:HE3	1:A:80:ASP:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLU:OE1	1:A:329:GLU:HA	2.08	0.53
1:B:226:PHE:CD2	1:B:279:PHE:HZ	2.26	0.53
1:A:33:ILE:HD12	1:A:33:ILE:N	2.24	0.53
1:B:230:ARG:CG	1:B:230:ARG:NH1	2.57	0.53
1:A:251:LEU:HD23	1:A:262:VAL:HG22	1.91	0.52
1:B:240:LYS:H	1:B:240:LYS:CE	2.23	0.51
1:A:73:VAL:HG23	1:A:314:LEU:HD12	1.93	0.51
1:B:28:ARG:CD	1:B:33:ILE:HD13	2.30	0.51
1:A:106:LYS:HG2	1:A:119:GLN:NE2	2.25	0.51
1:B:283:THR:O	1:B:284:ASP:HB2	2.10	0.51
1:B:268:VAL:HG12	1:B:270:PRO:HD3	1.93	0.51
1:A:139:GLU:OE1	1:B:124:LYS:CB	2.58	0.50
1:A:106:LYS:HG2	1:A:119:GLN:HE22	1.77	0.50
1:A:224:ARG:HD3	1:A:252:SER:HB2	1.93	0.49
1:A:231:ARG:HA	1:A:245:LYS:O	2.13	0.49
1:B:198:ALA:O	1:B:260:ILE:HD13	2.13	0.49
1:B:58:TYR:CB	1:B:82:GLY:O	2.59	0.49
1:A:287:ILE:HD13	1:A:314:LEU:HD11	1.94	0.49
1:A:269:VAL:HG11	1:A:272:HIS:ND1	2.29	0.48
1:A:276:SER:HB3	1:A:328:ILE:HG22	1.94	0.48
1:B:39:VAL:HG23	1:B:60:LYS:HB3	1.97	0.46
1:A:280:ILE:HD12	1:A:287:ILE:CG2	2.45	0.46
1:B:31:ALA:O	1:B:67:SER:HA	2.16	0.46
1:A:65:THR:HG23	1:A:74:ALA:HB3	1.98	0.46
1:B:15:ASN:HB3	1:B:16:TRP:H	1.60	0.46
1:B:130:ILE:HG23	1:B:130:ILE:O	2.15	0.46
1:A:215:SER:HG	1:A:277:PHE:HD2	1.62	0.46
1:B:162:GLU:HG2	1:B:173:GLU:HG2	1.97	0.46
1:B:300:VAL:CG2	1:B:324:LYS:HD3	2.46	0.45
1:B:66:LEU:HD22	1:B:280:ILE:HG21	1.99	0.45
1:A:29:THR:HB	1:A:30:PRO:HD2	1.98	0.44
1:B:49:ALA:HB3	1:B:54:THR:HB	1.98	0.44
1:A:130:ILE:O	1:A:130:ILE:HG23	2.18	0.44
1:A:89:ALA:O	1:B:88:LEU:HD12	2.18	0.44
1:B:299:ARG:O	1:B:299:ARG:HG3	2.18	0.44
1:B:147:LEU:HD22	1:B:154:LEU:HD11	2.01	0.43
1:A:280:ILE:HD12	1:A:287:ILE:HG22	2.00	0.43
1:B:126:VAL:HA	1:B:127:PRO:HD2	1.89	0.43
1:A:230:ARG:NH1	1:A:230:ARG:CG	2.48	0.43
1:B:50:GLN:HE21	1:B:50:GLN:HB2	1.52	0.42
1:B:214:GLU:CD	1:B:230:ARG:HD2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLY:HA3	1:A:189:HIS:CE1	2.54	0.42
1:B:280:ILE:HA	1:B:281:PRO:HD3	1.95	0.42
1:A:146:TRP:HB3	1:A:215:SER:HA	2.01	0.42
1:B:238:SER:OG	1:B:241:ASP:OD1	2.22	0.42
1:B:280:ILE:HD12	1:B:287:ILE:HG22	2.01	0.42
1:B:288:ILE:O	1:B:306:ALA:HA	2.20	0.42
1:B:324:LYS:HE3	1:B:324:LYS:HB2	1.69	0.42
1:B:150:LYS:HB3	1:B:155:TYR:CE2	2.55	0.41
1:A:112:ASP:HB2	1:A:143:LYS:HG2	2.01	0.41
1:B:64:LEU:C	1:B:64:LEU:HD23	2.40	0.41
1:B:93:ARG:NH1	1:B:113:ARG:NH1	2.69	0.41
1:B:146:TRP:CE2	1:B:157:GLY:HA3	2.55	0.41
1:B:238:SER:HB2	1:B:240:LYS:HE3	2.02	0.41
1:A:49:ALA:HB3	1:A:51:GLU:HB2	2.03	0.41
1:B:200:ARG:CZ	1:B:207:PRO:HG3	2.52	0.40
1:B:331:ILE:H	1:B:331:ILE:HG12	1.60	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	313/339 (92%)	299 (96%)	13 (4%)	1 (0%)	41	55
1	B	315/339 (93%)	295 (94%)	19 (6%)	1 (0%)	41	55
All	All	628/678 (93%)	594 (95%)	32 (5%)	2 (0%)	41	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	297	SER
1	A	296	ASP

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	265/283 (94%)	240 (91%)	25 (9%)	8	13
1	B	267/283 (94%)	234 (88%)	33 (12%)	4	5
All	All	532/566 (94%)	474 (89%)	58 (11%)	6	8

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	28	ARG
1	A	33	ILE
1	A	44	ASP
1	A	52	GLU
1	A	60	LYS
1	A	65	THR
1	A	71	ASP
1	A	79	LYS
1	A	101	ILE
1	A	132	SER
1	A	135	ASP
1	A	161	LYS
1	A	165	THR
1	A	173	GLU
1	A	179	LYS
1	A	194	SER
1	A	230	ARG
1	A	240	LYS
1	A	263	SER
1	A	294	GLU
1	A	299	ARG
1	A	305	MET
1	A	317	GLU
1	A	331	ILE
1	B	15	ASN
1	B	33	ILE

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Mol	Chain	Res	Type
1	B	50	GLN
1	B	59	LEU
1	B	66	LEU
1	B	71	ASP
1	B	76	GLU
1	B	79	LYS
1	B	84	LEU
1	B	93	ARG
1	B	101	ILE
1	B	124	LYS
1	B	151	ASP
1	B	169	ASP
1	B	179	LYS
1	B	186	SER
1	B	190	GLU
1	B	194	SER
1	B	230	ARG
1	B	233	SER
1	B	235	GLU
1	B	236	ARG
1	B	239	GLU
1	B	240	LYS
1	B	265	VAL
1	B	276	SER
1	B	282	ASN
1	B	299	ARG
1	B	302	SER
1	B	312	ARG
1	B	324	LYS
1	B	326	GLU
1	B	331	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	B	50	GLN
1	B	104	ASN
1	B	264	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](#)

Of 2 ligands modelled in this entry, 2 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	315/339 (92%)	-0.06	3 (0%) 82 80	27, 44, 59, 73	0
1	B	317/339 (93%)	0.08	6 (1%) 66 64	31, 47, 62, 70	0
All	All	632/678 (93%)	0.01	9 (1%) 75 73	27, 46, 61, 73	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	VAL	4.1
1	B	67	SER	3.0
1	A	331	ILE	3.0
1	A	71	ASP	2.9
1	A	166	THR	2.7
1	B	68	ASP	2.6
1	B	331	ILE	2.3
1	B	75	VAL	2.2
1	B	166	THR	2.1

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(\AA^2)	Q<0.9
2	CA	A	1000	1/1	0.95	0.06	47,47,47,47	0
2	CA	B	1001	1/1	0.95	0.16	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.