



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 03:29 PM EST

PDB ID : 3RQA
Title : The Crystal Structure of a Pathogenic Protein from the *Xanthomonas campestris* Reveals a New Tetrameric PilZ Domain Self-Assembled via a Un-usual Helical Bundle
Authors : Li, T.-N.; Chin, K.-H.; Chou, S.-H.
Deposited on : 2011-04-28
Resolution : 2.10 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
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

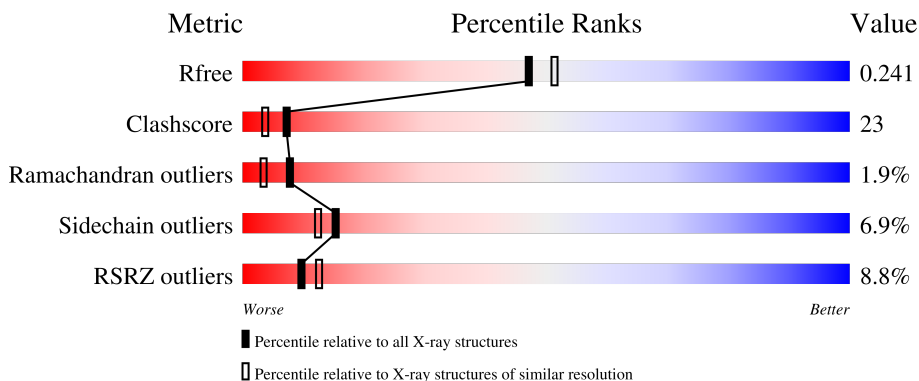
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	191	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 58%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 31%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">9% 58% 31% •• 8%</p>
1	B	191	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 51%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">9% 51% 29% 8% 12%</p>
1	C	191	<div style="display: flex; align-items: center;"> <div style="width: 11%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; 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: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">11% 65% 24% • 6%</p>
1	D	191	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3% 70% 16% • 12%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	B	1004	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5729 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	175	1349	853	247	247	2	0	0	0
1	B	168	1295	822	237	234	2	0	0	0
1	C	179	1375	868	251	253	3	0	0	0
1	D	169	1299	822	238	237	2	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP B0RT03
A	-1	ASN	-	expression tag	UNP B0RT03
A	0	ALA	-	expression tag	UNP B0RT03
B	-2	SER	-	expression tag	UNP B0RT03
B	-1	ASN	-	expression tag	UNP B0RT03
B	0	ALA	-	expression tag	UNP B0RT03
C	-2	SER	-	expression tag	UNP B0RT03
C	-1	ASN	-	expression tag	UNP B0RT03
C	0	ALA	-	expression tag	UNP B0RT03
D	-2	SER	-	expression tag	UNP B0RT03
D	-1	ASN	-	expression tag	UNP B0RT03
D	0	ALA	-	expression tag	UNP B0RT03

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0

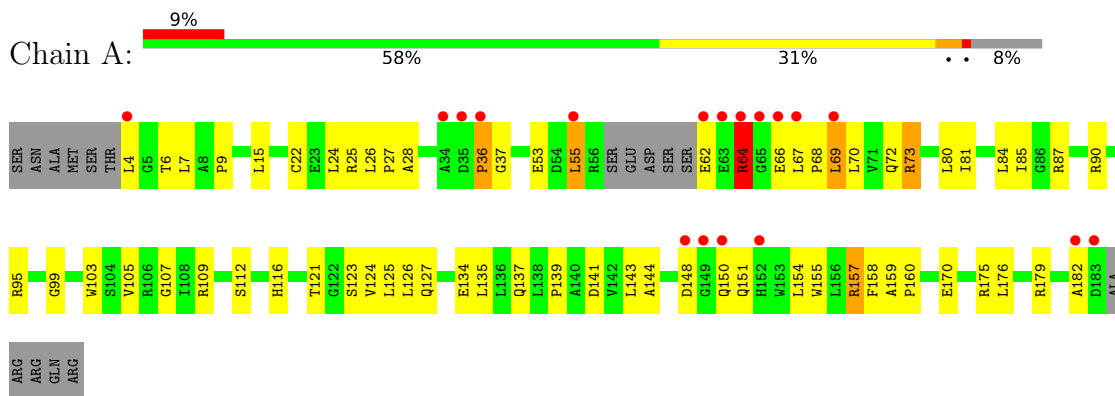
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	87	Total O 87 87	0	0
3	B	86	Total O 86 86	0	0
3	C	128	Total O 128 128	0	0
3	D	94	Total O 94 94	0	0

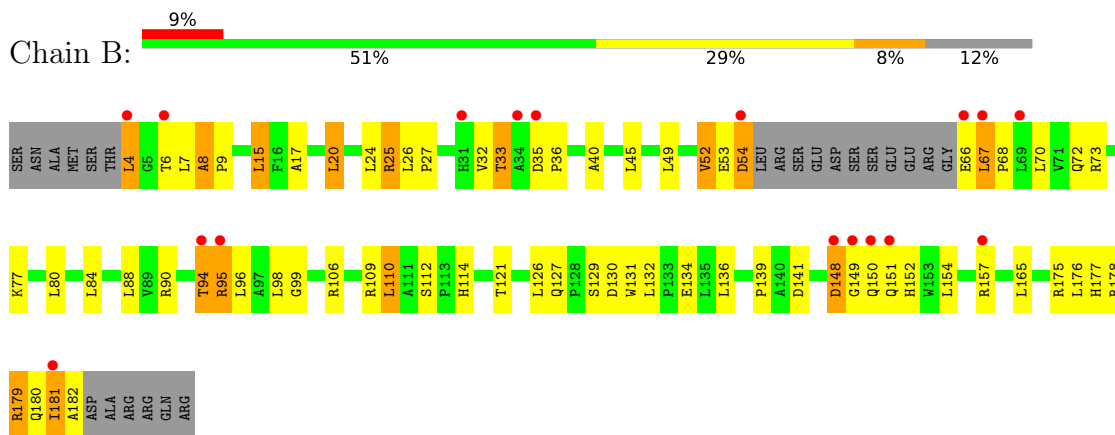
3 Residue-property plots [i](#)

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.

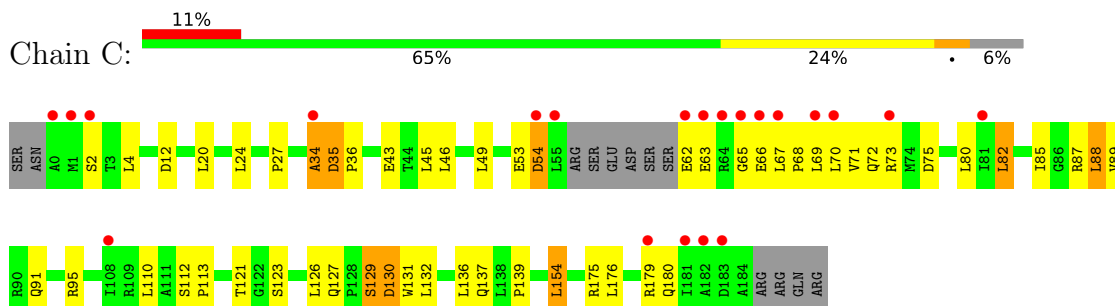
- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein

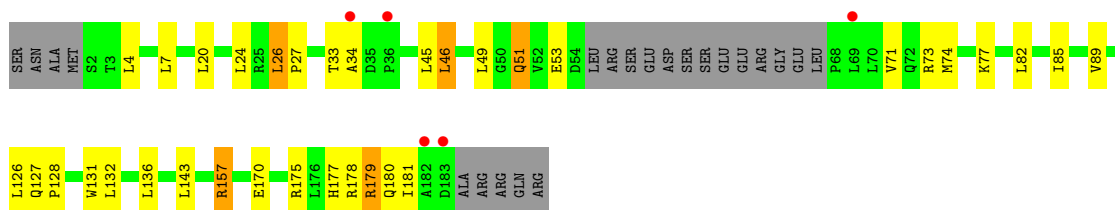


- Molecule 1: Putative uncharacterized protein



● Molecule 1: Putative uncharacterized protein

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.84Å 89.36Å 87.34Å 90.00° 105.40° 90.00°	Depositor
Resolution (Å)	25.02 – 2.10 25.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.1 (25.02-2.10) 99.4 (25.01-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.10Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.251 0.241 , 0.241	Depositor DCC
R_{free} test set	2564 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtrriage
Anisotropy	0.133	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5729	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: ACT

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	0.34	0/1378	0.63	0/1879
1	B	0.35	0/1324	0.67	0/1807
1	C	0.37	0/1404	0.66	0/1914
1	D	0.37	0/1328	0.62	0/1812
All	All	0.36	0/5434	0.64	0/7412

There are no bond length outliers.

There are no bond angle outliers.

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	1349	0	1354	76	0
1	B	1295	0	1309	94	0
1	C	1375	0	1386	59	0
1	D	1299	0	1309	38	0
2	A	8	0	6	1	0
2	B	4	0	3	1	0
2	C	4	0	3	1	0
3	A	87	0	0	3	0
3	B	86	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	128	0	0	7	0
3	D	94	0	0	3	0
All	All	5729	0	5370	241	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 23.

All (241) 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:95:ARG:HG3	1:B:95:ARG:HH11	1.19	1.07
1:A:64:ARG:H	1:A:64:ARG:NE	1.59	0.99
1:A:64:ARG:HE	1:A:64:ARG:N	1.63	0.96
1:C:35:ASP:H	1:C:36:PRO:HD3	1.25	0.95
1:A:90:ARG:HH11	1:A:95:ARG:HH12	1.09	0.95
1:C:27:PRO:HG2	1:C:127:GLN:HB3	1.47	0.95
1:C:73:ARG:NH1	1:D:51:GLN:HG3	1.83	0.93
1:C:36:PRO:HG2	1:C:139:PRO:HG3	1.51	0.90
1:A:70:LEU:HD22	1:B:66:GLU:HB2	1.51	0.90
1:C:73:ARG:HH11	1:D:51:GLN:HG3	1.31	0.90
1:A:36:PRO:HG2	1:A:37:GLY:H	1.38	0.88
1:B:25:ARG:H	1:B:25:ARG:HD2	1.38	0.88
1:A:27:PRO:HG2	1:A:127:GLN:HB3	1.55	0.88
1:A:73:ARG:HH11	1:A:73:ARG:HB2	1.39	0.87
1:C:35:ASP:N	1:C:36:PRO:HD3	1.88	0.86
1:A:80:LEU:HD22	1:B:132:LEU:HD21	1.58	0.85
1:A:69:LEU:HA	1:A:72:GLN:HE21	1.41	0.84
1:B:126:LEU:HD21	1:B:136:LEU:HD23	1.60	0.83
1:B:106:ARG:HD3	3:B:1011:HOH:O	1.78	0.82
1:B:178:ARG:HA	1:B:181:ILE:HG22	1.61	0.82
1:D:27:PRO:HG2	1:D:127:GLN:HB3	1.62	0.81
1:B:67:LEU:HB3	1:B:68:PRO:CD	2.10	0.81
1:B:67:LEU:HD12	1:B:67:LEU:H	1.47	0.80
1:A:90:ARG:NH1	1:A:95:ARG:HH12	1.80	0.79
1:A:73:ARG:HB2	1:A:73:ARG:NH1	1.97	0.78
1:B:70:LEU:HD23	1:C:67:LEU:HD22	1.66	0.77
1:A:68:PRO:HG2	1:B:67:LEU:HD21	1.65	0.77
1:C:35:ASP:H	1:C:36:PRO:CD	1.92	0.76
1:A:143:LEU:HD23	1:A:155:TRP:O	1.86	0.75
1:A:7:LEU:HD12	1:A:7:LEU:H	1.50	0.74
1:D:49:LEU:O	1:D:53:GLU:HG2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ARG:HH11	1:B:95:ARG:CG	1.99	0.73
1:B:179:ARG:HG2	1:B:179:ARG:HH21	1.53	0.72
2:B:1004:ACT:H2	3:B:367:HOH:O	1.89	0.72
1:A:143:LEU:HD22	1:A:157:ARG:HB2	1.71	0.72
1:C:129:SER:O	1:C:130:ASP:HB2	1.89	0.72
1:B:67:LEU:HB3	1:B:68:PRO:HD2	1.71	0.71
1:B:66:GLU:HB3	1:B:67:LEU:HD12	1.72	0.71
1:B:94:THR:O	1:B:95:ARG:HB2	1.92	0.70
1:C:36:PRO:HG3	1:C:123:SER:OG	1.91	0.70
1:C:73:ARG:HH11	1:D:51:GLN:CG	2.05	0.70
1:B:131:TRP:HZ2	3:B:209:HOH:O	1.75	0.68
1:D:71:VAL:HA	1:D:74:MET:HE2	1.76	0.68
1:A:7:LEU:H	1:A:7:LEU:CD1	2.08	0.67
1:A:73:ARG:HH11	1:A:73:ARG:CB	2.07	0.66
1:A:27:PRO:HG2	1:A:127:GLN:CB	2.25	0.66
1:C:34:ALA:HB1	1:C:36:PRO:HD3	1.78	0.65
1:A:73:ARG:NH2	1:B:54:ASP:O	2.30	0.65
1:C:180:GLN:HG3	3:C:288:HOH:O	1.97	0.65
1:B:88:LEU:HD21	1:C:89:VAL:HG22	1.79	0.64
1:A:124:VAL:HG12	1:A:126:LEU:HD13	1.80	0.63
1:A:175:ARG:HE	1:A:179:ARG:HH22	1.46	0.63
1:D:4:LEU:HA	1:D:7:LEU:HD23	1.79	0.63
1:D:175:ARG:O	1:D:179:ARG:HD3	1.98	0.63
1:B:179:ARG:HG2	1:B:179:ARG:NH2	2.11	0.63
1:B:165:LEU:O	1:B:165:LEU:HD12	1.99	0.62
1:C:35:ASP:N	1:C:36:PRO:CD	2.57	0.62
1:B:45:LEU:O	1:B:49:LEU:HD13	1.99	0.62
1:A:144:ALA:HB3	1:A:155:TRP:HB2	1.81	0.61
1:B:95:ARG:HG3	1:B:95:ARG:NH1	2.01	0.61
1:A:7:LEU:HD12	1:A:7:LEU:N	2.15	0.61
1:B:126:LEU:HD23	1:B:136:LEU:HB3	1.84	0.59
1:A:36:PRO:HG2	1:A:37:GLY:N	2.14	0.59
1:D:71:VAL:HA	1:D:74:MET:CE	2.32	0.59
1:D:33:THR:HG21	3:D:357:HOH:O	2.02	0.58
1:B:32:VAL:O	1:B:33:THR:HG23	2.02	0.58
1:C:176:LEU:HD23	1:C:179:ARG:HH22	1.68	0.58
1:D:131:TRP:CZ3	1:D:132:LEU:HD13	2.39	0.58
1:A:24:LEU:N	1:A:24:LEU:HD23	2.18	0.58
1:C:36:PRO:HA	1:C:137:GLN:HE21	1.69	0.58
1:B:67:LEU:HD12	1:B:67:LEU:N	2.19	0.57
1:A:6:THR:O	1:A:9:PRO:HD3	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LEU:HD12	1:B:26:LEU:O	2.05	0.57
1:D:131:TRP:CE3	1:D:132:LEU:HD13	2.39	0.57
1:A:90:ARG:HG2	1:A:95:ARG:HH22	1.68	0.57
1:B:4:LEU:C	1:B:6:THR:H	2.08	0.57
1:B:84:LEU:HD22	1:C:89:VAL:HG21	1.87	0.57
1:A:69:LEU:HA	1:A:72:GLN:NE2	2.17	0.57
1:B:67:LEU:H	1:B:67:LEU:CD1	2.16	0.56
1:A:22:CYS:SG	1:A:176:LEU:HD12	2.45	0.56
1:A:135:LEU:HD21	3:A:1019:HOH:O	2.04	0.56
1:B:7:LEU:HD23	1:B:7:LEU:H	1.71	0.56
1:B:24:LEU:HD13	1:B:176:LEU:HD21	1.87	0.56
1:B:25:ARG:HD2	1:B:25:ARG:N	2.14	0.56
1:B:148:ASP:O	1:B:150:GLN:N	2.34	0.56
1:C:36:PRO:HA	1:C:137:GLN:NE2	2.21	0.56
1:B:4:LEU:N	1:B:4:LEU:HD23	2.21	0.56
1:A:64:ARG:H	1:A:64:ARG:HE	0.77	0.56
1:C:67:LEU:HD11	1:C:71:VAL:HG11	1.87	0.56
1:A:121:THR:HG22	1:A:141:ASP:OD2	2.05	0.55
1:A:66:GLU:HG3	1:A:67:LEU:H	1.72	0.55
1:B:149:GLY:C	1:B:151:GLN:H	2.10	0.55
1:B:178:ARG:HG3	1:B:179:ARG:N	2.22	0.55
1:C:88:LEU:O	1:C:91:GLN:HB2	2.07	0.55
1:D:27:PRO:CG	1:D:127:GLN:HB3	2.36	0.55
1:A:170:GLU:HG2	3:A:237:HOH:O	2.06	0.55
1:B:127:GLN:HG2	1:B:129:SER:O	2.07	0.55
1:B:148:ASP:C	1:B:150:GLN:H	2.09	0.54
1:C:73:ARG:NH1	1:D:51:GLN:O	2.39	0.54
1:D:175:ARG:HG2	1:D:178:ARG:NH1	2.22	0.54
1:B:20:LEU:HD21	1:B:177:HIS:CD2	2.42	0.54
1:B:127:GLN:NE2	1:B:130:ASP:HA	2.23	0.54
1:D:33:THR:HG22	1:D:34:ALA:N	2.22	0.54
1:B:112:SER:HB3	1:B:154:LEU:HD13	1.89	0.53
1:B:36:PRO:HB2	1:B:139:PRO:HG3	1.89	0.53
1:A:62:GLU:HG2	3:D:222:HOH:O	2.08	0.53
1:A:143:LEU:HD23	1:A:143:LEU:H	1.73	0.53
1:C:121:THR:HB	3:C:230:HOH:O	2.07	0.53
1:B:131:TRP:CZ2	3:B:209:HOH:O	2.53	0.53
1:D:27:PRO:HG2	1:D:127:GLN:CB	2.38	0.53
1:A:36:PRO:HG2	1:A:139:PRO:HG3	1.90	0.53
1:C:45:LEU:O	1:C:49:LEU:HB2	2.08	0.53
1:A:84:LEU:HD11	1:B:132:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LEU:HB3	1:A:68:PRO:HD2	1.91	0.53
1:A:175:ARG:O	1:A:179:ARG:HG3	2.09	0.53
1:A:36:PRO:CG	1:A:37:GLY:H	2.12	0.53
1:B:181:ILE:HG23	1:B:181:ILE:O	2.08	0.52
1:B:24:LEU:HD23	1:B:24:LEU:N	2.24	0.52
1:B:84:LEU:HD11	1:C:132:LEU:HD11	1.92	0.52
1:B:25:ARG:H	1:B:25:ARG:CD	2.16	0.52
1:B:84:LEU:CD2	1:C:89:VAL:HG21	2.40	0.52
1:D:26:LEU:HD12	1:D:26:LEU:O	2.10	0.51
1:D:157:ARG:HH11	1:D:157:ARG:HG3	1.76	0.51
1:B:121:THR:HA	1:B:141:ASP:OD1	2.10	0.51
1:A:85:ILE:HD11	1:D:85:ILE:N	2.26	0.51
1:B:68:PRO:HG3	3:C:203:HOH:O	2.12	0.50
1:B:175:ARG:O	1:B:179:ARG:HD3	2.11	0.50
1:B:127:GLN:HE21	1:B:130:ASP:HA	1.76	0.50
1:B:53:GLU:HA	3:B:476:HOH:O	2.10	0.50
1:A:66:GLU:HG3	1:A:67:LEU:N	2.26	0.50
1:B:25:ARG:HB3	3:B:472:HOH:O	2.12	0.50
1:B:25:ARG:HA	1:B:99:GLY:O	2.10	0.50
1:B:17:ALA:O	1:B:106:ARG:NH2	2.39	0.50
1:B:52:VAL:HG23	1:B:52:VAL:O	2.11	0.50
1:C:112:SER:HB2	1:C:154:LEU:HD22	1.94	0.50
1:B:66:GLU:N	1:B:72:GLN:HG2	2.27	0.50
1:D:73:ARG:HH21	1:D:73:ARG:HG3	1.77	0.50
1:A:134:GLU:OE2	1:A:134:GLU:HA	2.12	0.49
1:B:150:GLN:O	1:B:151:GLN:NE2	2.45	0.49
1:C:129:SER:O	1:C:130:ASP:CB	2.59	0.49
3:B:397:HOH:O	1:C:43:GLU:HG2	2.13	0.49
1:B:27:PRO:HG2	1:B:127:GLN:HB3	1.94	0.49
1:D:177:HIS:NE2	1:D:181:ILE:HD11	2.28	0.48
1:A:67:LEU:HB3	1:A:68:PRO:CD	2.44	0.48
1:B:70:LEU:CD2	1:C:67:LEU:HD22	2.38	0.48
1:C:63:GLU:O	1:C:67:LEU:HB3	2.13	0.48
1:B:152:HIS:HB3	3:B:1010:HOH:O	2.14	0.48
1:C:176:LEU:HD23	1:C:179:ARG:NH2	2.29	0.48
1:C:175:ARG:NH1	3:C:204:HOH:O	2.47	0.48
1:A:15:LEU:HD22	1:A:107:GLY:HA3	1.94	0.48
1:A:176:LEU:C	1:A:176:LEU:HD13	2.34	0.47
1:B:8:ALA:N	1:B:9:PRO:CD	2.77	0.47
1:A:55:LEU:HD11	1:D:77:LYS:HZ1	1.78	0.47
1:A:81:ILE:O	1:A:85:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASP:C	1:B:150:GLN:N	2.67	0.47
1:B:179:ARG:HH21	1:B:179:ARG:CG	2.23	0.47
1:D:51:GLN:HE21	1:D:51:GLN:HB2	1.55	0.47
2:A:1003:ACT:H2	1:B:40:ALA:HB3	1.97	0.47
1:B:126:LEU:CD2	1:B:136:LEU:HB3	2.44	0.47
1:C:70:LEU:HD13	1:C:70:LEU:O	2.13	0.47
1:A:24:LEU:HD23	1:A:24:LEU:H	1.78	0.47
1:B:33:THR:HG21	3:B:1007:HOH:O	2.14	0.47
1:A:28:ALA:HB1	1:A:126:LEU:HD12	1.97	0.47
1:B:73:ARG:O	1:B:77:LYS:HG3	2.15	0.47
1:B:95:ARG:CG	1:B:95:ARG:NH1	2.66	0.47
1:B:70:LEU:HD11	1:C:75:ASP:OD1	2.14	0.46
1:A:175:ARG:HB3	1:A:179:ARG:NH1	2.30	0.46
1:C:82:LEU:O	1:C:85:ILE:HG22	2.15	0.46
1:C:87:ARG:HD2	1:D:89:VAL:HG11	1.97	0.46
1:A:73:ARG:HH21	1:B:54:ASP:H	1.63	0.46
1:D:170:GLU:HG2	3:D:197:HOH:O	2.16	0.46
1:A:90:ARG:NH1	1:A:95:ARG:NH1	2.57	0.46
1:D:46:LEU:HD13	1:D:136:LEU:HD13	1.98	0.45
1:A:36:PRO:CG	1:A:37:GLY:N	2.74	0.45
1:B:45:LEU:HD13	1:B:134:GLU:HG2	1.97	0.45
1:C:67:LEU:HD11	1:C:71:VAL:CG1	2.45	0.45
1:A:4:LEU:O	1:A:4:LEU:HG	2.16	0.45
1:A:116:HIS:HE1	3:A:524:HOH:O	1.99	0.45
1:B:70:LEU:HD23	1:C:67:LEU:CD2	2.43	0.45
1:C:63:GLU:HB2	1:C:72:GLN:HG2	1.99	0.45
1:C:46:LEU:HD13	1:C:136:LEU:HD13	1.98	0.45
1:A:80:LEU:HD21	1:B:49:LEU:HD12	1.98	0.45
1:A:157:ARG:HD3	1:A:158:PHE:O	2.16	0.45
1:A:73:ARG:CD	3:B:210:HOH:O	2.65	0.44
1:B:67:LEU:CB	1:B:68:PRO:CD	2.87	0.44
1:D:143:LEU:HG	1:D:157:ARG:HB2	1.99	0.44
1:B:26:LEU:HD12	1:B:26:LEU:C	2.38	0.44
1:B:114:HIS:HA	1:B:152:HIS:HD2	1.83	0.44
1:C:63:GLU:HG3	1:C:72:GLN:CD	2.38	0.44
1:D:45:LEU:O	1:D:49:LEU:HB2	2.17	0.44
1:A:25:ARG:HA	1:A:99:GLY:O	2.17	0.44
1:A:36:PRO:CB	1:A:123:SER:OG	2.65	0.44
1:B:150:GLN:HA	1:B:150:GLN:OE1	2.17	0.44
1:C:73:ARG:HH12	1:D:51:GLN:HA	1.83	0.44
1:D:49:LEU:HD12	1:D:49:LEU:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:HIS:O	1:D:181:ILE:HG13	2.17	0.44
1:A:7:LEU:HD21	1:A:148:ASP:HB3	2.01	0.43
1:A:28:ALA:HA	1:A:125:LEU:O	2.17	0.43
1:A:179:ARG:O	1:A:182:ALA:HB3	2.18	0.43
1:D:126:LEU:O	1:D:128:PRO:HD3	2.18	0.43
1:C:63:GLU:OE1	1:C:72:GLN:HB3	2.18	0.43
1:C:2:SER:OG	1:C:4:LEU:HD13	2.18	0.43
1:D:24:LEU:N	1:D:24:LEU:HD23	2.33	0.43
1:C:69:LEU:O	1:C:73:ARG:HD3	2.18	0.43
1:C:131:TRP:CD2	2:C:1002:ACT:H2	2.54	0.43
1:C:176:LEU:CD2	1:C:179:ARG:HH22	2.32	0.42
1:B:15:LEU:CD1	1:B:157:ARG:HD3	2.50	0.42
1:B:25:ARG:HH21	1:B:25:ARG:HG3	1.84	0.42
1:A:123:SER:HB3	1:A:137:GLN:HG3	2.02	0.42
1:A:124:VAL:CG1	1:A:126:LEU:HD13	2.48	0.42
1:B:90:ARG:HD3	3:B:339:HOH:O	2.18	0.42
1:A:36:PRO:HG3	1:A:123:SER:OG	2.18	0.42
1:B:27:PRO:HG2	1:B:127:GLN:CB	2.50	0.42
1:D:175:ARG:HG2	1:D:178:ARG:HH12	1.83	0.42
1:B:8:ALA:H	1:B:9:PRO:CD	2.33	0.42
1:C:65:GLY:O	1:C:66:GLU:HB3	2.19	0.41
1:C:112:SER:CB	1:C:154:LEU:HD22	2.49	0.41
1:D:73:ARG:O	1:D:77:LYS:HG3	2.20	0.41
1:D:82:LEU:O	1:D:85:ILE:HG22	2.20	0.41
1:A:80:LEU:HD22	1:B:132:LEU:CD2	2.38	0.41
1:B:180:GLN:C	1:B:182:ALA:H	2.24	0.41
1:C:24:LEU:N	1:C:24:LEU:HD23	2.35	0.41
1:A:105:VAL:HG22	1:A:105:VAL:O	2.21	0.41
1:A:159:ALA:O	1:A:160:PRO:C	2.59	0.41
1:A:84:LEU:HD11	1:B:132:LEU:CD1	2.51	0.41
1:A:109:ARG:HA	1:A:154:LEU:O	2.20	0.41
1:A:112:SER:HB2	1:A:154:LEU:HD12	2.03	0.41
1:B:4:LEU:C	1:B:6:THR:N	2.73	0.41
1:B:109:ARG:HG3	1:B:109:ARG:HH11	1.85	0.41
1:C:87:ARG:HD3	3:C:226:HOH:O	2.21	0.41
1:C:110:LEU:C	1:C:110:LEU:HD12	2.41	0.41
1:C:73:ARG:NE	3:C:1015:HOH:O	2.52	0.41
1:B:70:LEU:HD11	1:C:75:ASP:CG	2.41	0.41
1:C:49:LEU:HD11	1:C:129:SER:HB2	2.02	0.41
1:C:53:GLU:HB3	1:C:54:ASP:H	1.74	0.41
1:C:176:LEU:HD11	3:C:241:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TRP:CH2	1:A:126:LEU:HD23	2.57	0.40
1:C:112:SER:HA	1:C:113:PRO:HD3	1.96	0.40
1:B:110:LEU:O	1:B:110:LEU:HD12	2.21	0.40
1:D:53:GLU:OE1	1:D:53:GLU:HA	2.21	0.40
1:A:87:ARG:HH11	1:B:134:GLU:CD	2.23	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	171/191 (90%)	152 (89%)	16 (9%)	3 (2%)	8	4
1	B	164/191 (86%)	149 (91%)	10 (6%)	5 (3%)	4	1
1	C	175/191 (92%)	165 (94%)	5 (3%)	5 (3%)	4	1
1	D	165/191 (86%)	159 (96%)	6 (4%)	0	100	100
All	All	675/764 (88%)	625 (93%)	37 (6%)	13 (2%)	8	3

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	PRO
1	A	64	ARG
1	A	151	GLN
1	B	8	ALA
1	B	67	LEU
1	C	35	ASP
1	B	148	ASP
1	C	34	ALA
1	C	68	PRO
1	C	129	SER

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Mol	Chain	Res	Type
1	C	130	ASP
1	B	181	ILE
1	B	52	VAL

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	142/157 (90%)	134 (94%)	8 (6%)	21	18
1	B	137/157 (87%)	123 (90%)	14 (10%)	7	4
1	C	145/157 (92%)	135 (93%)	10 (7%)	15	12
1	D	138/157 (88%)	131 (95%)	7 (5%)	24	22
All	All	562/628 (90%)	523 (93%)	39 (7%)	15	12

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	53	GLU
1	A	55	LEU
1	A	64	ARG
1	A	69	LEU
1	A	73	ARG
1	A	150	GLN
1	A	157	ARG
1	B	4	LEU
1	B	15	LEU
1	B	20	LEU
1	B	25	ARG
1	B	33	THR
1	B	35	ASP
1	B	54	ASP
1	B	80	LEU
1	B	94	THR
1	B	95	ARG

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Mol	Chain	Res	Type
1	B	96	LEU
1	B	98	LEU
1	B	110	LEU
1	B	179	ARG
1	C	12	ASP
1	C	20	LEU
1	C	54	ASP
1	C	62	GLU
1	C	80	LEU
1	C	82	LEU
1	C	88	LEU
1	C	95	ARG
1	C	126	LEU
1	C	154	LEU
1	D	20	LEU
1	D	26	LEU
1	D	46	LEU
1	D	51	GLN
1	D	157	ARG
1	D	179	ARG
1	D	180	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	91	GLN
1	A	150	GLN
1	B	51	GLN
1	B	91	GLN
1	B	116	HIS
1	B	127	GLN
1	B	137	GLN
1	B	151	GLN
1	C	72	GLN
1	C	137	GLN
1	C	152	HIS
1	D	51	GLN
1	D	91	GLN
1	D	116	HIS
1	D	152	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](#)

4 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	$\# Z > 2$
2	ACT	A	1001	-	3,3,3	0.09	0	3,3,3	0.62	0
2	ACT	B	1004	-	3,3,3	0.08	0	3,3,3	0.62	0
2	ACT	A	1003	-	3,3,3	0.08	0	3,3,3	0.62	0
2	ACT	C	1002	-	3,3,3	0.09	0	3,3,3	0.63	0

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1004	ACT	1	0
2	A	1003	ACT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1002	ACT	1	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

6.1 Protein, DNA and RNA chains

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	175/191 (91%)	0.54	18 (10%) 6 8	23, 44, 82, 118	0
1	B	168/191 (87%)	0.68	17 (10%) 7 9	25, 49, 77, 90	0
1	C	179/191 (93%)	0.50	21 (11%) 4 6	19, 35, 82, 99	0
1	D	169/191 (88%)	0.06	5 (2%) 50 56	19, 34, 68, 86	0
All	All	691/764 (90%)	0.45	61 (8%) 10 12	19, 39, 77, 118	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	54	ASP	8.0
1	C	1	MET	7.1
1	A	62	GLU	6.7
1	B	150	GLN	6.6
1	C	55	LEU	6.3
1	B	4	LEU	6.0
1	D	183	ASP	5.8
1	A	63	GLU	5.4
1	B	181	ILE	5.4
1	C	0	ALA	5.2
1	B	151	GLN	4.9
1	C	64	ARG	4.6
1	A	64	ARG	4.4
1	C	62	GLU	4.4
1	C	67	LEU	4.3
1	A	4	LEU	4.1
1	B	149	GLY	4.1
1	C	66	GLU	4.1
1	C	34	ALA	3.9
1	A	55	LEU	3.7
1	C	63	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	2	SER	3.5
1	B	69	LEU	3.4
1	D	182	ALA	3.4
1	A	69	LEU	3.4
1	C	182	ALA	3.3
1	C	65	GLY	3.3
1	C	69	LEU	3.2
1	B	34	ALA	3.2
1	A	65	GLY	3.1
1	A	36	PRO	3.1
1	A	67	LEU	3.0
1	D	69	LEU	3.0
1	D	36	PRO	3.0
1	B	67	LEU	2.8
1	C	108	ILE	2.8
1	B	66	GLU	2.8
1	B	6	THR	2.8
1	A	150	GLN	2.8
1	A	35	ASP	2.7
1	B	95	ARG	2.7
1	A	34	ALA	2.6
1	C	183	ASP	2.6
1	C	73	ARG	2.6
1	C	181	ILE	2.5
1	A	182	ALA	2.5
1	A	183	ASP	2.5
1	A	148	ASP	2.4
1	A	149	GLY	2.3
1	B	148	ASP	2.3
1	A	66	GLU	2.2
1	B	35	ASP	2.2
1	A	152	HIS	2.2
1	C	81	ILE	2.2
1	B	54	ASP	2.2
1	B	94	THR	2.2
1	D	34	ALA	2.1
1	B	31	HIS	2.1
1	C	70	LEU	2.1
1	B	157	ARG	2.1
1	C	179	ARG	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	ACT	B	1004	4/4	0.72	0.55	10,13,14,15	0
2	ACT	C	1002	4/4	0.85	0.31	10,13,14,15	0
2	ACT	A	1003	4/4	0.86	0.35	10,13,14,15	0
2	ACT	A	1001	4/4	0.90	0.33	10,13,14,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.